



# STIC Search Report

EIC 1700

STIC Database Tracking Number: 09/485533

**TO:** Rabon A Sergeant  
**Location:** REM 10D65  
**Art Unit :** 1711  
**December 28, 2005**

**Case Serial Number:** 09/485533

**From:** Usha Shrestha  
**Location:** EIC 1700  
**REMSEN 4B28**  
**Phone:** 571/272-3519  
**usha.shrestha@uspto.gov**

Search Notes

=> fil reg  
FILE 'REGISTRY' ENTERED AT 13:15:17 ON 28 DEC 2005

=> d his

FILE 'HCAPLUS' ENTERED AT 08:17:15 ON 28 DEC 2005  
L1 1 S WO1998-FR01800/PRN,AP  
SEL RN

FILE 'REGISTRY' ENTERED AT 08:18:23 ON 28 DEC 2005  
L2 12 S E1-E12  
L3 889 S 4.264.1/RID  
L4 15227 S 46.492.1/RID  
E URETDIONE  
E URETIDINEDIONE/CN  
E URETIDIONE/CN  
E URETDIONE/CN  
L5 1 S E10  
L6 71218 S PUR/PCT  
L7 2 S L2 AND L6  
L8 162 S L3 AND L6  
L9 7609 S L6 NOT 1-50/NR  
L10 1 S 220652-25-5/RN  
L11 1 S 220588-31-8/RN  
L12 245445 S OTHER/PCT  
L13 81225 S OTHERO/PCT  
L14 245445 S L12 OR L13  
L15 2 S L14 AND L2  
L16 68 S L14 AND L3  
L17 98094 S L14 NOT 2-100/NR  
L18 8 S L17 AND L3  
L19 4617 S PIR/PCT  
L20 0 S L19 AND L2  
L21 339 S L19 NOT 1-100/NR  
L22 154 S L3 NOT 2-100/NR  
L23 42 S L19 AND L3  
L24 1 S L23 NOT 2-100/NR  
L25 10 S L8 NOT 2-100/NR

FILE 'HCAPLUS' ENTERED AT 12:10:19 ON 28 DEC 2005  
L26 734 S L3  
L27 5 S L18  
L28 1 S L24  
L29 5 S L25  
L30 9 S L27-L29  
L31 323 S L26 (L) PREP/RL  
L32 82 S L31 (L) (?URETHAN? OR ?ISOCYANAT?)  
L33 32 S L32 AND (HEAT? OR TEMP?)  
L34 12 S L33 NOT CAT?  
L35 242 S L31 NOT CAT?  
L36 68 S L35 AND (HEAT? OR TEMP?)  
L37 24 S L32 AND CAT/RL  
L38 58 S L32 NOT L37  
L39 17 S L38 AND (HEAT? OR TEMP?)

FILE 'REGISTRY' ENTERED AT 12:30:34 ON 28 DEC 2005  
L40 154 S L3 NOT 2-100/NR

FILE 'HCAPLUS' ENTERED AT 12:31:05 ON 28 DEC 2005  
L41 180 S L40

L42 77 S L41(L) PREP/RL  
 L43 27 S L42(L) (?URETHAN? OR ?ISOCYANAT?)  
 L44 54 S L42 AND (?URETHAN? OR ?ISOCYANAT?)  
 L45 13 S L44 AND CAT?/RL  
 L46 41 S L44 NOT L45  
 L47 18 S L46 AND (HEAT? OR TEMP?)  
 L48 1 S L47 AND L1  
 L49 27 S L30 OR L47  
 L50 46 S L46 OR L47 OR L49

=> d que 150

L3 889 SEA FILE=REGISTRY ABB=ON PLU=ON 4.264.1/RID  
 L6 71218 SEA FILE=REGISTRY ABB=ON PLU=ON PUR/PCT  
 L8 162 SEA FILE=REGISTRY ABB=ON PLU=ON L3 AND L6  
 L12 245445 SEA FILE=REGISTRY ABB=ON PLU=ON OTHER/PCT  
 L13 81225 SEA FILE=REGISTRY ABB=ON PLU=ON OTHERO/PCT  
 L14 245445 SEA FILE=REGISTRY ABB=ON PLU=ON L12 OR L13  
 L17 98094 SEA FILE=REGISTRY ABB=ON PLU=ON L14 NOT 2-100/NR  
 L18 8 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND L3  
 L19 4617 SEA FILE=REGISTRY ABB=ON PLU=ON PIR/PCT  
 L23 42 SEA FILE=REGISTRY ABB=ON PLU=ON L19 AND L3  
 L24 1 SEA FILE=REGISTRY ABB=ON PLU=ON L23 NOT 2-100/NR  
 L25 10 SEA FILE=REGISTRY ABB=ON PLU=ON L8 NOT 2-100/NR  
 L27 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L18  
 L28 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L24  
 L29 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L25  
 L30 9 SEA FILE=HCAPLUS ABB=ON PLU=ON (L27 OR L28 OR L29)  
 L40 154 SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT 2-100/NR  
 L41 180 SEA FILE=HCAPLUS ABB=ON PLU=ON L40  
 L42 77 SEA FILE=HCAPLUS ABB=ON PLU=ON L41(L) PREP/RL  
 L44 54 SEA FILE=HCAPLUS ABB=ON PLU=ON L42 AND (?URETHAN? OR  
     ?ISOCYANAT?)  
 L45 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L44 AND CAT?/RL  
 L46 41 SEA FILE=HCAPLUS ABB=ON PLU=ON L44 NOT L45  
 L47 18 SEA FILE=HCAPLUS ABB=ON PLU=ON L46 AND (HEAT? OR  
     TEMP?)  
 L49 27 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 OR L47  
 L50 46 SEA FILE=HCAPLUS ABB=ON PLU=ON L46 OR L47 OR L49

=> fil hcap

FILE 'HCAPLUS' ENTERED AT 13:15:35 ON 28 DEC 2005

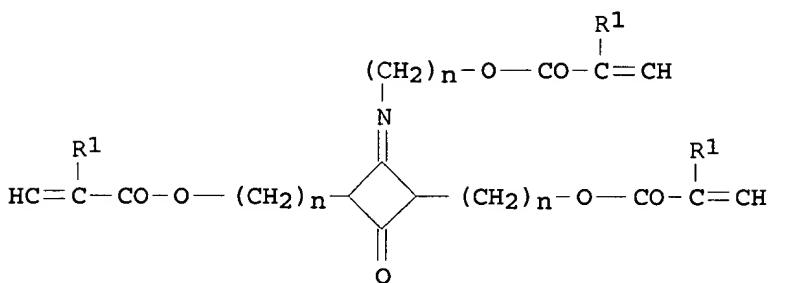
=> => d 150 1-46 ibib abs hitstr hitind

L50 ANSWER 1 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2005:405056 HCAPLUS  
 DOCUMENT NUMBER: 142:433133  
 TITLE: Urethonimines bearing double bonds, their  
       polymers, gels, ion-conductive compositions,  
       and their applications  
 INVENTOR(S): Aizawa, Wakana; Iida, Kazuyuki  
 PATENT ASSIGNEE(S): Mitsubishi Paper Mills, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.             | KIND | DATE           | APPLICATION NO. | DATE         |
|------------------------|------|----------------|-----------------|--------------|
| JP 2005119969          | A2   | 20050512       | JP 2003-353147  | 2003<br>1014 |
| PRIORITY APPLN. INFO.: |      | JP 2003-353147 |                 | 2003<br>1014 |

OTHER SOURCE(S): MARPAT 142:433133  
 GI



AB The urethonimines are I ( $\text{R}^1 = \text{H}$ , alkyl;  $n = 2-6$ ). The urethonimines are polymerized in various solvents without undesired side reactions between carbodiimide groups and active H. The polymers, useful as electrolytes for electrochem. devices, e.g., secondary Li batteries, capacitors, and surface modifiers, show good heat resistance because they generate isocyanate and carbodiimide groups suppressing hydrolysis.

IT 850789-28-5P 850789-29-6P 850789-30-9P  
 850789-32-1P

(urethonimines bearing double bonds for ion-conductive polymer gels showing good heat resistance for secondary Li batteries, double-layer capacitors, and surface modifiers)

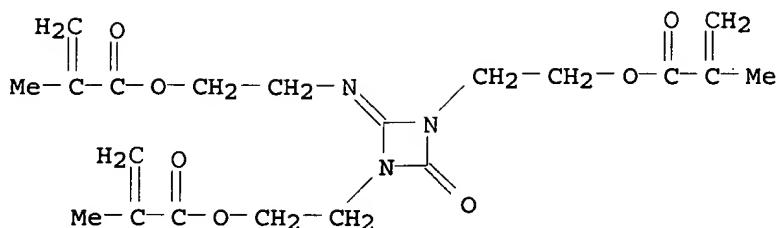
RN 850789-28-5 HCPLUS

CN 2-Propenoic acid, 2-methyl-, methanetetraylbis(nitrilo-2,1-ethanediyl) ester, polymer with [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidine-1,3-diyl]di-2,1-ethanediyl bis(2-methyl-2-propenoate) (9CI) (CA INDEX NAME)

CM 1

CRN 850789-27-4

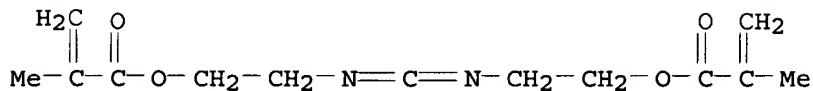
CMF C20 H27 N3 O7



CM 2

CRN 817619-67-3

CMF C13 H18 N2 O4



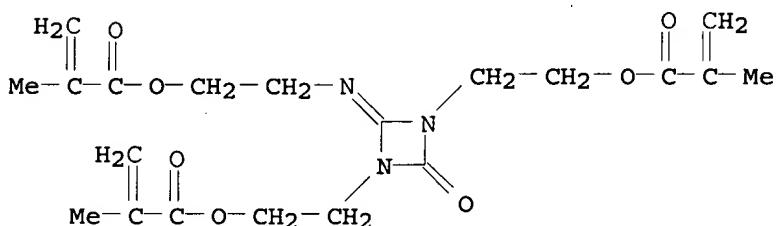
RN 850789-29-6 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidine-1,3-diyli]di-2,1-ethanediyl ester, polymer with  $\alpha$ -(2-methyl-1-oxo-2-propenyl)- $\omega$ -methoxypoly(oxy-1,2-ethanediyl) (9CI) (CA INDEX NAME)

CM 1

CRN 850789-27-4

CMF C20 H27 N3 O7

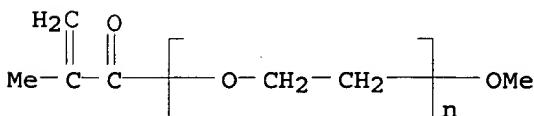


CM 2

CRN 26915-72-0

CMF (C2 H4 O)n C5 H8 O2

CCI PMS



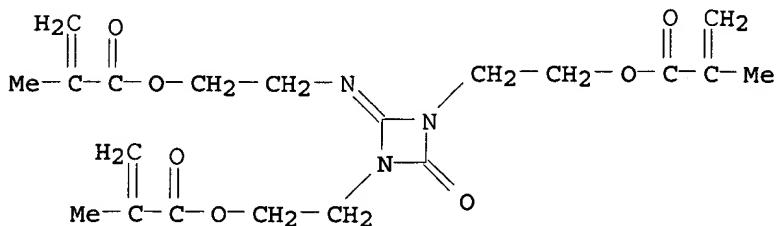
RN 850789-30-9 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidine-1,3-diyl]di-2,1-ethanediyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 850789-27-4

CMF C20 H27 N3 O7



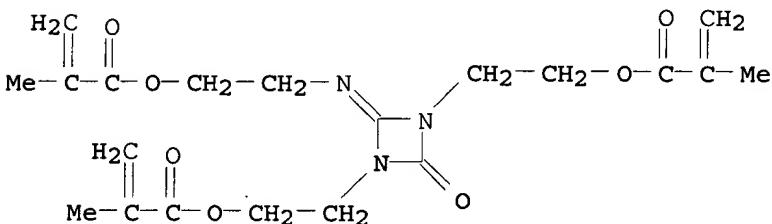
RN 850789-32-1 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidine-1,3-diyl]di-2,1-ethanediyl ester, polymer with ethene, graft (9CI) (CA INDEX NAME)

CM 1

CRN 850789-27-4

CMF C20 H27 N3 O7



CM 2

CRN 74-85-1

CMF C2 H4

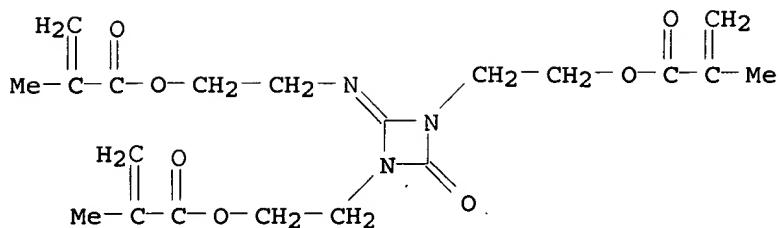
H<sub>2</sub>C=CH<sub>2</sub>

IT 850789-27-4P

(urethonimines bearing double bonds for ion-conductive polymer gels showing good heat resistance for secondary Li batteries, double-layer capacitors, and surface modifiers)

RN 850789-27-4 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidinediyl]di-2,1-ethanediyl ester (9CI) (CA INDEX NAME)



IT 850789-31-0P

(urethonimines bearing double bonds for ion-conductive polymer gels showing good heat resistance for secondary Li batteries, double-layer capacitors, and surface modifiers)

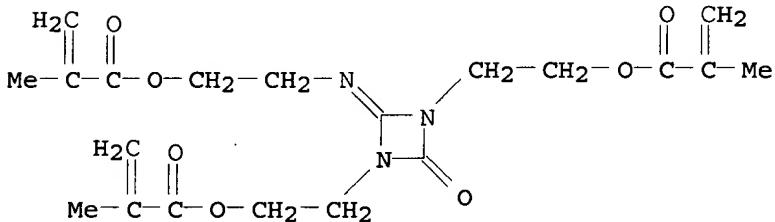
RN 850789-31-0 HCPLUS

CN 2-Propenoic acid, 2-methyl-, methanetetraylbis(nitrilo-2,1-ethanediyl) ester, polymer with [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidine-1,3-diyli]di-2,1-ethanediyl bis(2-methyl-2-propenoate) and  $\alpha$ -(1-oxo-2-propenyl)- $\omega$ -methoxypoly(oxy-1,2-ethanediyl) (9CI). (CA INDEX NAME)

CM 1

CRN 850789-27-4

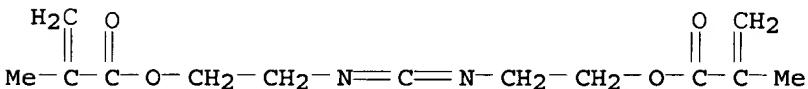
CMF C20 H27 N3 O7



CM 2

CRN 817619-67-3

CMF C13 H18 N2 O4

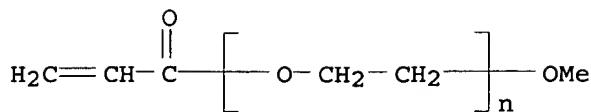


CM 3

CRN 32171-39-4

CMF (C2 H4 O)n C4 H6 O2

CCI PMS



IC ICM C07D229-00  
 ICS C08F020-36; C08F291-00; C08F292-00; H01G009-038; H01M010-40  
 CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)  
 Section cross-reference(s): 28, 35, 38, 76  
 ST urethonimine polymer ionic conductor **heat** resistance;  
 lithium battery urethonimine polymer gel electrolyte; capacitor  
 urethonimine polymer gel electrolyte; surface modifier  
 urethonimine polymer  
 IT Polyoxalkylenes, uses  
 (acrylic, urethonimine-containing; urethonimines bearing double  
 bonds for ion-conductive polymer gels showing good **heat**  
 resistance for secondary Li batteries, double-layer capacitors,  
 and surface modifiers)  
 IT Capacitors  
 (double layer; urethonimines bearing double bonds for  
 ion-conductive polymer gels showing good **heat**  
 resistance for secondary Li batteries, double-layer capacitors,  
 and surface modifiers)  
 IT Secondary batteries  
 (lithium; urethonimines bearing double bonds for ion-conductive  
 polymer gels showing good **heat** resistance for  
 secondary Li batteries, double-layer capacitors, and surface  
 modifiers)  
 IT Surface treatment  
 (modifiers; urethonimines bearing double bonds for  
 ion-conductive polymer gels showing good **heat**  
 resistance for secondary Li batteries, double-layer capacitors,  
 and surface modifiers)  
 IT Ionic conductors  
 (polymeric; urethonimines bearing double bonds for  
 ion-conductive polymer gels showing good **heat**  
 resistance for secondary Li batteries, double-layer capacitors,  
 and surface modifiers)  
 IT Electrolytic capacitors  
 Gels  
 Heat-resistant materials  
 Polymer electrolytes  
 (urethonimines bearing double bonds for ion-conductive polymer  
 gels showing good **heat** resistance for secondary Li  
 batteries, double-layer capacitors, and surface modifiers)  
 IT 850789-28-5P 850789-29-6P 850789-30-9P  
 850789-32-1P  
 (urethonimines bearing double bonds for ion-conductive polymer  
 gels showing good **heat** resistance for secondary Li  
 batteries, double-layer capacitors, and surface modifiers)  
 IT 817619-67-3P 850789-27-4P  
 (urethonimines bearing double bonds for ion-conductive polymer  
 gels showing good **heat** resistance for secondary Li  
 batteries, double-layer capacitors, and surface modifiers)  
 IT 850789-31-0P  
 (urethonimines bearing double bonds for ion-conductive polymer  
 gels showing good **heat** resistance for secondary Li  
 batteries, double-layer capacitors, and surface modifiers)  
 IT 30674-80-7

(urethonimines bearing double bonds for ion-conductive polymer gels showing good heat resistance for secondary Li batteries, double-layer capacitors, and surface modifiers)

L50 ANSWER 2 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:20011 HCAPLUS

DOCUMENT NUMBER: 140:78231

TITLE: Pressure-sensitive acrylic adhesives without foaming nor substrate staining and polarizing films therewith showing good processability

INVENTOR(S): Ebata, Norimitsu; Miyazaki, Hideki; Nakagawa, Nobuo; Uemae, Masami

PATENT ASSIGNEE(S): Nippon Carbide Industries Co., Inc., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.             | KIND  | DATE     | APPLICATION NO. | DATE              |
|------------------------|-------|----------|-----------------|-------------------|
| -----                  | ----- | -----    | -----           | -----             |
| -----                  | ----- | -----    | -----           | -----             |
| JP 2004002782          | A2    | 20040108 | JP 2003-98425   | 2003<br>0401      |
| PRIORITY APPLN. INFO.: |       |          | JP 2002-103154  | A<br>2002<br>0405 |

AB The adhesives comprise (A) high-mol.-weight acrylic copolymers [Mw 900,000-2,500,000, Tg  $\leq$  -45°, SP 8.7-9.3 (SP = solubility parameter)] having reactive functional groups 100, (B) low-mol.-weight acrylic copolymers (Mw 50,000-200,000, Tg -40 to 0°, SP 8.7-9.3) prepared from (b1) H2C:CHCO2R1 [R1 = C4-10 (branched) alkyl] whose homopolymers satisfy Tg  $\leq$  -50°, (b2) monomers relatively less copolymerizable with b1, and (b3) monomers relatively highly copolymerizable with b1 5-100, and (C) polyfunctional compds. crosslinkable with A 0.001-10 parts. Thus, acrylic acid-n-Bu acrylate (BA) copolymer (Mw 1,200,000, Tg -55°, SP 9.1) was mixed with BA-n-Bu methacrylate-Me acrylate copolymer (Mw 90,000, Tg -15°, SP 9.1) and Duranate E 405-80T (modified HMDI) to give an adhesive composition, which was applied on a release film, laminated with poly(vinyl alc.)/cellulose triacetate polarizing film, and dried to give adhesive layer-equipped film. The film was bonded on a glass sheet showing 180° peel strength 450 and 700 g/25 mm, after aging at 23° and 70°, resp., no foaming nor light-leaking defect after 1000-h aging at 100°, and no glass staining after peeling.

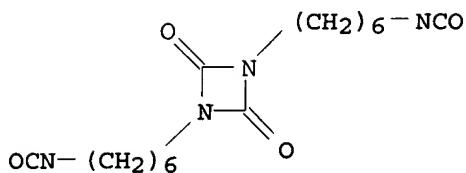
IT 641636-24-0P  
(pressure-sensitive acrylic adhesives without foaming nor substrate staining useful for polarizing films)

RN 641636-24-0 HCAPLUS

CN 2-Propenoic acid, polymer with 1,3-bis(6-isocyanatohexyl)-1,3-diazetidine-2,4-dione and butyl 2-propenoate (9CI) (CA INDEX NAME)

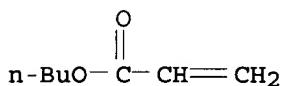
CM 1

CRN 23501-81-7  
CMF C16 H24 N4 O4



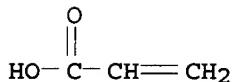
CM 2

CRN 141-32-2  
CMF C7 H12 O2



CM 3

CRN 79-10-7  
CMF C3 H4 O2



IC ICM C09J133-08  
ICS C09J133-02; C09J133-10; C09J163-00; C09J175-04; C09J183-08  
CC 38-3 (Plastics Fabrication and Uses)  
Section cross-reference(s): 73, 74  
IT 77-99-6DP, Trimethylolpropane, reaction products with (hydrogenated) xylylene **diisocyanate** or HMDI, polymers with acrylic acid copolymers 822-06-0DP, HMDI, modified, polymers with acrylic acid copolymers 25854-16-4DP, Xylylene **diisocyanate**, reaction products with trimethylolpropane, polymers with acrylic acid-n-Bu acrylate-2-hydroxyethyl acrylate copolymer 42170-25-2DP, reaction products with trimethylolpropane, polymers with acrylic acid-n-Bu acrylate copolymer 152048-77-6P, Acrylic acid-n-butyl acrylate-TETRAD-C copolymer 416844-24-1P 416844-36-5P, Acrylic acid-n-butyl acrylate-Desmodur N 3400 copolymer 556818-60-1P, Acrylic acid-butyl acrylate-Takenate D 120N copolymer 556818-63-4P, Acrylic acid-n-butyl acrylate-Coronate HX copolymer 641620-83-9P, Acrylic acid-n-butyl acrylate-Duranate E 405-80T copolymer 641620-84-0P 641620-85-1P 641620-86-2P 641620-87-3P, Acrylic acid-n-butyl acrylate-Coronate HL-S copolymer 641620-88-4P, Acrylic acid-butyl acrylate-2-ethylhexyl acrylate-methyl acrylate-Takenate M 631N copolymer 641620-89-5P, Acrylic acid-butyl acrylate-ethyl acrylate-Duranate E 405-80T-2-ethylhexyl acrylate copolymer 641620-90-8P, Acrylic

acid-butyl acrylate-Duranate E 405-80T-methyl methacrylate copolymer 641636-19-3P, Acrylic acid-n-butyl acrylate-hexamethylene diisocyanate isocyanurate copolymer 641636-24-0P  
(pressure-sensitive acrylic adhesives without foaming nor substrate staining useful for polarizing films)

L50 ANSWER 3 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:359890 HCAPLUS

DOCUMENT NUMBER: 136:355793

TITLE: **Diisocyanatononane-based polyisocyanates**

INVENTOR(S): Suzuki, Shigeaki; Hori, Hiroshi

PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.  
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

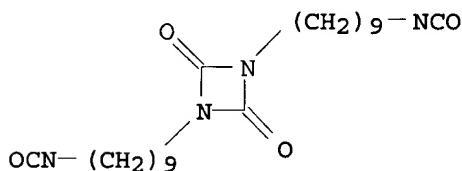
| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------|
| JP 2002138129          | A2   | 20020514 | JP 2000-335981  | 2000 |
|                        |      |          |                 | 1102 |
| PRIORITY APPLN. INFO.: |      |          | JP 2000-335981  | 2000 |
|                        |      |          |                 | 1102 |

AB The **polyisocyanates** are manufactured by either of (a) biuret formation of 1,9-diisocyanatononane (I) or 1,8-diisocyanato-2-methyloctane (II), (b) reaction of I or II with polyol, or (c) cyclodimerization of I or II. I and II show low vapor pressure and the **polyisocyanates** show high reactivity. Thus, I was treated with H<sub>2</sub>O in the presence of Me<sub>3</sub>PO<sub>4</sub> to give biuret **polyisocyanate**.

IT 420135-71-3P 420789-42-0P  
(manufacture of **diisocyanatononane-based polyisocyanates**)

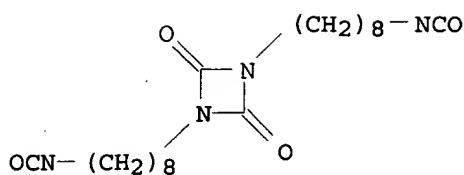
RN 420135-71-3 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(9-isocyanatononyl)- (9CI) (CA INDEX NAME)



RN 420789-42-0 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis[8-isocyanato-2(or 7)-methyloctyl]- (9CI) (CA INDEX NAME)



2 (D1-Me)

IC ICM C08G018-73  
 ICS C08G018-10  
 CC 37-2 (Plastics Manufacture and Processing)  
 ST isocyanatononane polyisocyanate manuf; biuret  
 polyisocyanate diisocyanatononane manuf; polyol  
 diisocyanatononane adduct polyisocyanate manuf;  
 cyclodimerization diisocyanatononane  
 polyisocyanate manuf  
 IT 420135-69-9P 420135-70-2P  
 (biuret-type, oligomeric; manufacture of diisocyanatononane  
 -based polyisocyanates)  
 IT 77-99-6DP, Trimethylolpropane, reaction products with  
 diisocyanato(iso)nonane 7192-79-2DP, reaction products  
 with trimethylolpropane 176506-52-8DP, reaction products with  
 trimethylolpropane 420135-71-3P 420789-42-0P  
 (manufacture of diisocyanatononane-based  
 polyisocyanates)  
 IT 7192-79-2 176506-52-8  
 (manufacture of diisocyanatononane-based  
 polyisocyanates)

L50 ANSWER 4 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:711613 HCAPLUS

DOCUMENT NUMBER: 136:69773

TITLE: Synthesis of N-functionalized carbodiimides,  
 hydantoins, 1,3-diazetidines, and  
 imidazolidine derivatives from N-vinylic  
 phosphazenes derived from  $\beta$ -amino acids  
 Palacios, Francisco; Legido, Marta; Perez de  
 Heredia, Itziar; Ezpeleta, Jose Maria;  
 Rubiales, Gloria

AUTHOR(S):

CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de  
 Farmacia, Universidad del Pais Vasco, Vitoria,  
 01080, SpainSOURCE: Heterocycles (2001), 55(9), 1641-1651  
 CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:69773

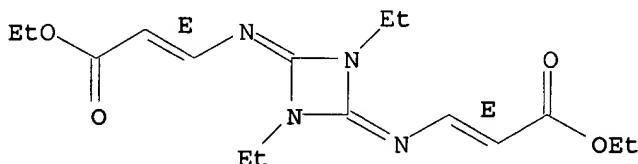
AB Synthesis of N-vinylic carbodiimides through aza-Wittig reaction  
 of N-vinylic phosphazenes with isocyanates is reported.  
 These heterocumulenes are used for the preparation of unsym. ureas and  
 nitrogen heterocycles such as hydantoins, 1,3-diazetidines,  
 imidazolidinones, and bis-imidazolidinone azines.IT 384372-45-6P 384372-46-7P  
 (preparation of N-functionalized carbodiimides, hydantoins,

1,3-diazetidines, and imidazolidine derivs. from N-vinylic phosphazenes derived from  $\beta$ -amino acids)

RN 384372-45-6 HCPLUS

CN 2-Propenoic acid, 3,3'-(1,3-diethyl-1,3-diazetidine-2,4-diyldene)dinitriolo]bis-, diethyl ester, (2E,2'E)- (9CI) (CA INDEX NAME)

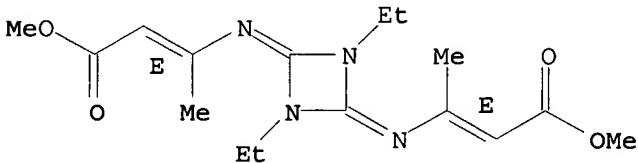
Double bond geometry as shown.



RN 384372-46-7 HCPLUS

CN 2-Butenoic acid, 3,3'-(1,3-diethyl-1,3-diazetidine-2,4-diyldene)dinitriolo]bis-, dimethyl ester, (2E,2'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

ST carbodiimide deriv prep hydration; hydantoin deriv prep; diazetidine deriv prep; imidazolidine deriv prep; phosphazene vinylic reaction **isocyanate**

IT 103-71-9, Phenyl **isocyanate**, reactions 109-90-0, Ethyl **isocyanate** 110-78-1, Propyl **isocyanate**

81777-30-2 152975-95-6 152975-96-7 384372-48-9 384372-49-0  
384372-51-4 421598-34-7

(preparation of N-functionalized carbodiimides, hydantoins, 1,3-diazetidines, and imidazolidine derivs. from N-vinylic phosphazenes derived from  $\beta$ -amino acids)

IT 384372-39-8P 384372-40-1P 384372-41-2P 384372-42-3P

384372-44-5P 384372-45-6P 384372-46-7P

384372-47-8P 384372-50-3P 384842-74-4P 384842-75-5P

384842-76-6P 384842-77-7P 384842-78-8P

(preparation of N-functionalized carbodiimides, hydantoins, 1,3-diazetidines, and imidazolidine derivs. from N-vinylic phosphazenes derived from  $\beta$ -amino acids)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 5 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:581955 HCPLUS

DOCUMENT NUMBER: 135:153862

TITLE: Preparation of two component polyurethane foam compositions for sound and vibration absorbers

INVENTOR(S): Bicknell, Rodney; Kirkham, Helen; Spencer,

PATENT ASSIGNEE(S): Richard  
 Baxenden Chemicals Limited, UK  
 SOURCE: PCT Int. Appl., 23 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE         |
|---|------|----------|-----------------|--------------|
| WO 2001057107   | A1   | 20010809 | WO 2001-GB408   | 2001<br>0131 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA,<br>CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD,<br>GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR,<br>KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,<br>MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,<br>TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,<br>AZ, BY, KG, KZ, MD, RU, TJ, TM |      |          |                 |              |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE,<br>CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,<br>PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR,<br>NE, SN, TD, TG   |      |          |                 |              |
| EP 1254187  | A1   | 20021106 | EP 2001-948990  | 2001<br>0131 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,<br>MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  |      |          |                 |              |
| US 2003119929   | A1   | 20030626 | US 2002-182678  | 2002<br>0903 |
| PRIORITY APPLN. INFO.:  |      |          | GB 2000-2175    | A            |
|   |      |          |                 | 2000<br>0131 |
|   |      |          | WO 2001-GB408   | W            |
|   |      |          |                 | 2001<br>0131 |

AB The process comprises mixing (A) a polyol resin component, (B) an isocyanate component having a free monomeric diisocyanate content of  $\leq 2$  wt%, and (C) a catalyst blend comprising  $\geq 2$  catalytic materials selected from (a) organometallic catalysts, (b) amines, and (c) isocyanurate catalysts. Thus a polyurethane foam was prepared by mixing of polyoxypropylated glycerol, polyoxypropylated toluene diamine, polyoxypropylene diol, diethanolamine, B 8404, triethylene glycol diamine, dibutyltin dilaurate, Baxcat 0, tri(3-dimethylaminopropyl)amine, hexamethylene diisocyanate biuret, and propylene carbonate with tetrafluoroethane, showing core d. 100-120 kg/m<sup>3</sup>, closed cell content (ASTM D2856) 3.6%, and flammability 3.05 cm/min (1.2 in./min) determined by MVSS-320 test.

IT 353245-35-9P 353245-36-0P  
 (preparation of two component polyurethane foam compns. for sound and vibration absorbers)

RN 353245-35-9 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer

with Castomer E 1004,  $\alpha$ -hydro- $\omega$ -hydroxypoly[oxy(methyl-1,2-ethanediyl)] and  $\alpha, \alpha', \alpha''$ -1,2,3-propanetriyltris[ $\omega$ -hydroxypoly[oxy(methyl-1,2-ethanediyl)]] (9CI) (CA INDEX NAME)

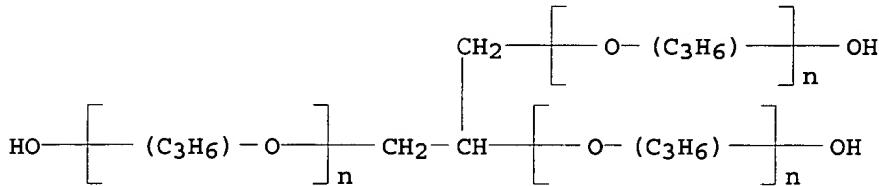
CM 1

CRN 353244-60-7  
CMF Unspecified  
CCI PMS, MAN

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

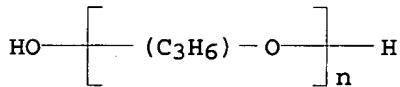
CM 2

CRN 25791-96-2  
CMF  $(C_3 H_6 O)_n$   $(C_3 H_6 O)_n$   $(C_3 H_6 O)_n$   $C_3 H_8 O_3$   
CCI IDS, PMS



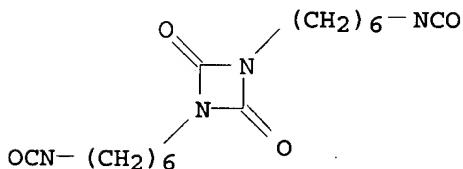
CM 3

CRN 25322-69-4  
CMF  $(C_3 H_6 O)_n$   $H_2 O$   
CCI IDS, PMS



CM 4

CRN 23501-81-7  
CMF  $C_{16} H_{24} N_4 O_4$



RN 353245-36-0 HCPLUS  
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with Castomer E 1004,  $\alpha$ -hydro- $\omega$ -hydroxypoly(oxy-1,2-

ethanediyl) and  $\alpha, \alpha', \alpha''$ -1,2,3-propanetriyltris[ $\omega$ -hydroxypoly[oxy(methyl-1,2-ethanediyl)]] (9CI) (CA INDEX NAME)

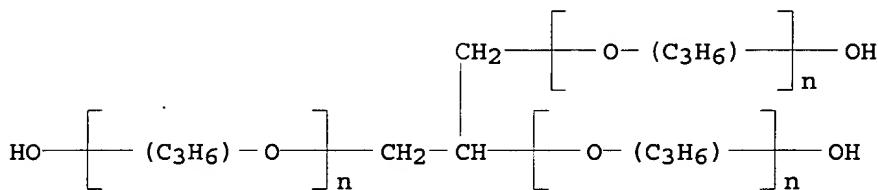
CM 1

CRN 353244-60-7  
CMF Unspecified  
CCI PMS, MAN

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

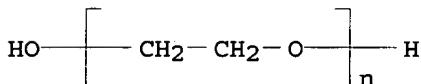
CM 2

CRN 25791-96-2  
CMF  $(C_3 H_6 O)_n$   $(C_3 H_6 O)_n$   $(C_3 H_6 O)_n$   $C_3 H_8 O_3$   
CCI IDS, PMS



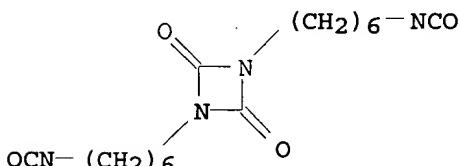
CM 3

CRN 25322-68-3  
CMF  $(C_2 H_4 O)_n$   $H_2 O$   
CCI PMS



CM 4

CRN 23501-81-7  
CMF  $C_{16} H_{24} N_4 O_4$



IC ICM C08G018-16  
CC 38-3 (Plastics Fabrication and Uses)  
Section cross-reference(s): 29, 67  
IT 4035-89-6DP, Hexamethylene diisocyanate biuret, polymers with

Mannich base and polyoxypropylated glycerol 23501-81-7DP, polymers with Mannich base, polyoxypropylated glycerol, and TDI prepolymer 25791-96-2DP, polymers with Mannich base, hexamethylene diisocyanate uretdione, and TDI prepolymer 26471-62-5DP, TDI, polymers with Mannich base, polyoxypropylated glycerol, and hexamethylene diisocyanate uretdione 352205-41-5P 352205-43-7P 353244-60-7P, Castomer E 1004 353245-35-9P  
**353245-36-0P**

(preparation of two component polyurethane foam compns. for sound and vibration absorbers)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 6 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:439337 HCAPLUS

DOCUMENT NUMBER: 131:89112

TITLE: Reducing volatile organic content of coating compositions by using a ketimine of acetone

INVENTOR(S): Richards, Bradley M.; Dantiki, Sudhakar

PATENT ASSIGNEE(S): BASF Corporation, USA

SOURCE: U.S., 5 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

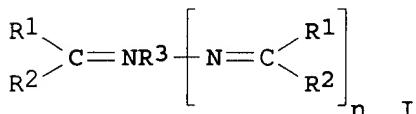
PATENT INFORMATION:

| PATENT NO. | KIND  | DATE     | APPLICATION NO. | DATE  |
|------------|-------|----------|-----------------|-------|
| -----      | ----- | -----    | -----           | ----- |
| -----      | ----- | -----    | -----           | ----- |
| US 5922804 | A     | 19990713 | US 1996-672800  | 1996  |

PRIORITY APPLN. INFO.: US 1996-672800

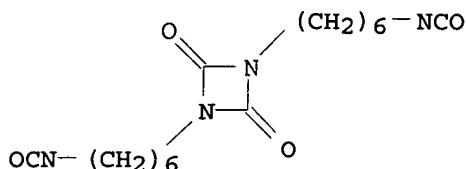
1996  
0628

GI



AB The volatile organic content of coating compns. is reduced by forming the ketimine of acetone by reacting acetone and a ketimine I, where  $n = 1-4$ ;  $\text{R}^1, \text{R}^2$  are (sep.) alkyl, aryl, cycloaliph. or substituted alkyl, aryl, or cycloaliph. group, except both  $\text{R}^1$  and  $\text{R}^2 \neq \text{Me}$ ;  $\text{R}^3$  is an aliphatic, aromatic, arylaliph., or cycloaliph. group, which can also contain O, N, S or Si. The ketimine of acetone is subsequently reacted with at least one isocyanate functional crosslinking resin. Thus, 62.2 g uretdione polyisocyanate was added to a 50:50 solution of diketimine and acetone, and the coating sprayed on cold-rolled

IT steel panels, giving dry film thickness 2.6 mil, dust-free drying time 60 s, and tack-free drying time 105 s.  
23501-81-7DP, Hexamethylene diisocyanate dimer, polymers with ketimines and hydroxy-functional resins (reducing volatile organic content of coating compns. by using a ketimine of acetone)  
RN 23501-81-7 HCAPLUS  
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl) - (9CI) (CA INDEX NAME)



IC ICM C08L075-02  
ICs C08L075-04; C08G018-10  
INCL 524589000  
CC 42-5 (Coatings, Inks, and Related Products)  
ST coating VOC redn acetone ketimine; **isocyanate**  
crosslinker acetone ketimine polyol  
IT 23501-81-7DP, Hexamethylene **diisocyanate** dimer,  
polymers with ketimines and hydroxy-functional resins  
(reducing volatile organic content of coating compns. by using a  
ketimine of acetone)  
IT 584-84-9D, Toluene 2,4-**diisocyanate**, polymers with  
ketimines and hydroxy-functional resins 822-06-0D, HMDI,  
polymers with ketimines and hydroxy-functional resins  
1014-98-8D, p-Xylene **diisocyanate**, polymers with  
ketimines and hydroxy-functional resins 3173-72-6D,  
1,5-Naphthalene **diisocyanate**, polymers with ketimines  
and hydroxy-functional resins 3634-83-1D, m-Xylylene  
**diisocyanate**, polymers with ketimines and  
hydroxy-functional resins 4098-71-9D, Isophorone  
**diisocyanate**, polymers with ketimines and  
hydroxy-functional resins 5124-30-1D, 4,4'-  
**Diisocyanatodicyclohexylmethane**, polymers with ketimines  
and hydroxy-functional resins 10581-16-5D, 1-Methyl-2,4-  
**diisocyanatocyclohexane**, polymers with ketimines and  
hydroxy-functional resins 25626-25-9D, Benzene, 1,2-bis(  
**isocyanatomethyl**), polymers with ketimines and  
hydroxy-functional resins  
(reducing volatile organic content of coating compns. by using a  
ketimine of acetone)

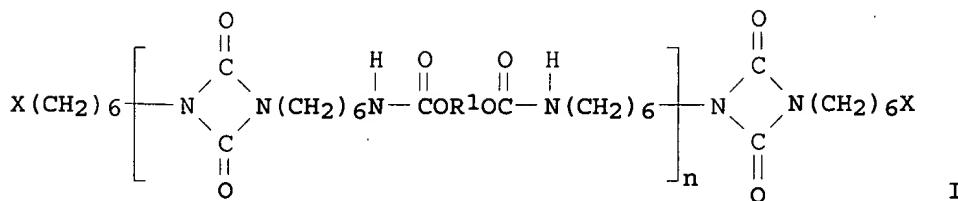
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 7 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1999:157156 HCAPLUS  
DOCUMENT NUMBER: 130:244437  
TITLE: Electrophotographic toner containing  
polyisocyanate  
INVENTOR(S): Ibuki, Ichiro; Hamatsu, Takao  
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.             | KIND | DATE           | APPLICATION NO. | DATE         |
|------------------------|------|----------------|-----------------|--------------|
| JP 11065169            | A2   | 19990305       | JP 1997-219483  | 1997<br>0814 |
| PRIORITY APPLN. INFO.: |      | JP 1997-219483 |                 | 1997<br>0814 |

GI

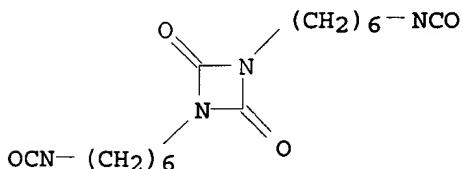


AB The toner comprises a polyol resin and a colorant as a main component and further a **polyisocyanate** containing a linear crystalline polyuretdione I [X = NHCO<sub>2</sub>R<sub>2</sub>OH, NHC(O)R<sub>3</sub>, NCO; R<sub>1</sub> = R<sub>2</sub>, R<sub>2</sub>O<sub>2</sub>CNR<sub>4</sub>NHCO<sub>2</sub>R<sub>2</sub>; R<sub>2</sub> = diol residue; R<sub>3</sub> = residue of a compound having 1 active H; R<sub>4</sub> = **diisocyanate** residue; n ≥ 1] with 8-21 weight% of potential NCO%, 2000-20,000 weight average mol. weight, and 60-140° m.p. The toner shows low **temperature fixability** and no offset.

IT 23501-81-7DP, polymer with ethylene glycol and polyester-polyol  
 (electrophotog. toner containing polyuretdione-derived polyurethanes with low **temperature fixability** and offset resistance)

RN 23501-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



IC ICM G03G009-087

CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

Section cross-reference(s): 35

ST electrophotog toner **polyisocyanate** polyol

polyuretodione; low **temp** fixability offset resistance toner

IT Electrophotographic toners  
(electrophotog. toner containing polyuretodione-derived polyurethanes with low **temperature** fixability and offset resistance)

IT Polyurethanes, uses  
(electrophotog. toner containing polyuretodione-derived polyurethanes with low **temperature** fixability and offset resistance)

IT Acrylic polymers, preparation  
(hydroxy-containing, polymer with polyuretodione; electrophotog. toner containing polyuretodione-derived polyurethanes with low **temperature** fixability and offset resistance)

IT Polyesters, preparation  
(polymers with hexamethylene diisocyanate polyuretodiones and ethylene glycol; electrophotog. toner containing polyuretodione-derived polyurethanes with low **temperature** fixability and offset resistance)

IT 100-42-5DP, Styrene, hydroxy-containing acrylic resin, polymer with polyuretodione 107-21-1DP, Ethylene glycol, polymer with hexamethylene diisocyanate polyuretodione and polyester-polyols 23501-81-7DP, polymer with ethylene glycol and polyester-polyol  
(electrophotog. toner containing polyuretodione-derived polyurethanes with low **temperature** fixability and offset resistance)

L50 ANSWER 8 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:126953 HCAPLUS  
 DOCUMENT NUMBER: 130:183894  
 TITLE: Method for preparing (poly)isocyanate compositions with reduced viscosity and their use in the manufacture of polyurethane coatings  
 INVENTOR(S): Charriere, Eugenie; Bernard, Jean-Marie; Revelant, Denis; Randu, Stephane  
 PATENT ASSIGNEE(S): Rhodia Chimie, Fr.  
 SOURCE: PCT Int. Appl., 67 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.  | KIND  | DATE     | APPLICATION NO. | DATE         |
|---|-------|----------|-----------------|--------------|
| -----   | ----- | -----    | -----           | -----        |
| -----   | ----- | -----    | -----           | -----        |
| WO 9907765  | A1    | 19990218 | WO 1998-FR1800  | 1998<br>0812 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU,<br>CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL,<br>IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,<br>MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,<br>SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW<br>RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE,<br>DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF,<br>BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG |       |          |                 |              |
| FR 2767328  | A1    | 19990219 | FR 1997-10296   |              |

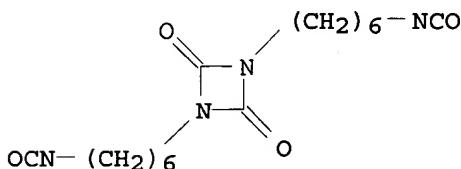
|  |    |                 |      |
|--|----|-----------------|------|
| FR 2767328   | B1 | 20010622        | 1997 |
| FR 2779142   | A1 | 19991203        | 0812 |
|  |    | FR 1998-6849    |      |
| FR 2779142   | B1 | 20000818        | 1998 |
| CA 2301071   | AA | 19990218        | 0529 |
|  |    | CA 1998-2301071 |      |
| AU 9890758   | A1 | 19990301        | 1998 |
|  |    | AU 1998-90758   | 0812 |
| AU 757808  | B2 | 20030306        | 1998 |
| ZA 9807209   | A  | 20000214        | 0812 |
|  |    | ZA 1998-7209    |      |
| EP 1003802   | A1 | 20000531        | 1998 |
|  |    | EP 1998-942735  | 0812 |
| EP 1003802   | B1 | 20041222        | 1998 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,<br>MC, PT, IE, FI     |    |                 | 0812 |
| BR 9811904   | A  | 20000815        |      |
|  |    | BR 1998-11904   |      |
| EP 1466931   | A2 | 20041013        | 1998 |
|  |    | EP 2004-14335   | 0812 |
| EP 1466931   | A3 | 20051102        | 1998 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,<br>MC, PT, IE, FI, CY |    |                 | 0812 |
| AT 285426  | E  | 20050115        |      |
|  |    | AT 1998-942735  |      |
| ES 2230713   | T3 | 20050501        | 1998 |
|  |    | ES 1998-942735  | 0812 |
| US 2004106762  | A1 | 20040603        | 2003 |
|  |    | US 2003-682412  | 1010 |
| PRIORITY APPLN. INFO.:   |    | FR 1997-10296   | A    |
|  |    |                 | 1997 |
|  |    |                 | 0812 |
|  |    | FR 1998-6849    | A    |
|  |    |                 | 1998 |
|  |    |                 | 0529 |
|  |    | EP 1998-942735  | A3   |
|  |    |                 | 1998 |
|  |    |                 | 0812 |
|  |    | WO 1998-FR1800  | W    |
|  |    |                 | 1998 |
|  |    |                 | 0812 |
|  |    | US 2000-485533  | A1   |
|  |    |                 | 2000 |
|  |    |                 | 0609 |

AB The invention concerns a method for preparing a (poly) isocyanate composition with reduced viscosity comprising at least dimers with uretidinedione group from initial monomeric isocyanates, characterized in that the initial reaction medium is heated, in the absence of a dimerization catalyst, at 50-200° for ≤24 h. When trimerization catalysts are present, the products also contain trimers, and, when polyols such as pentaerythritol and trimethylolpropane are present, the products contain carbamate group-containing prepolymers. The products are storage stable and have Hazen color value <100.

IT 23501-81-7P, Hexamethylene diisocyanate dimer (preparing polyisocyanate compns. containing diisocyanate dimers with reduced viscosity for use in manufacture of polyurethane coatings)

RN 23501-81-7 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)

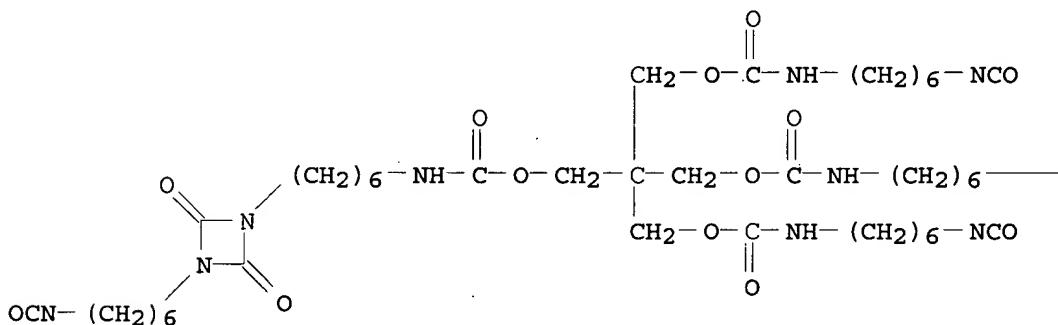


IT 220588-32-9P (preparing polyisocyanate compns. containing diisocyanate dimers with reduced viscosity for use in manufacture of polyurethane coatings)

RN 220588-32-9 HCPLUS

CN Carbamic acid, (6-isocyanatohexyl)-, 2-[[[[[6-isocyanatohexyl]amino]carbonyl]oxy]methyl]-2-[[[[[6-[3-(6-isocyanatohexyl)-2,4-dioxo-1,3-diazetidin-1-yl]hexyl]amino]carbonyl]oxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— NCO

IC ICM C08G018-79  
 ICS C08G018-32; C08G018-42; C08G018-62  
 CC 42-10 (Coatings, Inks, and Related Products)  
 ST uretidinedione **diisocyanate** dimer manuf dimerization catalyst absence; trimethylolpropane uretidinedione dimer adduct manuf; pentaerythritol uretidinedione dimer adduct manuf; **polyurethane** coating uretidinedione **diisocyanate** dimer precursor manuf  
 IT **Polyurethanes**, uses (acrylic; preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)  
 IT Acrylic polymers, uses (**polyurethane**; preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)  
 IT Coating materials (preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)  
 IT **Polyurethanes**, uses (preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)  
 IT 220652-25-5P 220652-27-7P (cured coating; preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)  
 IT 30228-08-1P (in preparation of IPDI dimer; preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)  
 IT 53895-31-1P (preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)  
 IT 3779-63-3P, Hexamethylene **diisocyanate** trimer  
 23501-81-7P, Hexamethylene **diisocyanate** dimer (preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)  
 IT 4035-89-6P 220588-31-8P 220588-32-9P 220588-33-0P  
 220617-22-1P, 1,3-Bis(isocyanatonorbornyl)-1,3-diazetidine-2,4-dione (preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)  
 IT 30322-28-2P, Hexamethylene **diisocyanate**-trimethylolpropane copolymer

(prepolymers, in preparation of HDI dimer; preparing polyisocyanate compns. containing diisocyanate dimers with reduced viscosity for use in manufacture of polyurethane coatings)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 9 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998:379199 HCPLUS  
 DOCUMENT NUMBER: 129:55022  
 TITLE: Uretdione group-containing polyaddition compounds and procedure for their production  
 INVENTOR(S): Gras, Rainer; Wolf, Elmar  
 PATENT ASSIGNEE(S): Huels A.-G., Germany  
 SOURCE: Ger. Offen., 6 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.             | KIND  | DATE     | APPLICATION NO.  | DATE  |
|------------------------|-------|----------|------------------|-------|
| -----                  | ----- | -----    | -----            | ----- |
| -----                  | ----- | -----    | -----            | ----- |
| DE 19650043            | A1    | 19980604 | DE 1996-19650043 | 1996  |
|                        |       |          |                  | 1203  |
| PRIORITY APPLN. INFO.: |       |          | DE 1996-19650043 | 1996  |
|                        |       |          |                  | 1203  |

AB Title compds., useful as storage-stable curing agents for polyurethane powders, are manufactured by reaction of uretdiones of HDI, 2-methylpentamethylene diisocyanate, or 2,2,4(2,4,4)-trimethylhexamethylene diisocyanate with R1NHROH [I, R1 = H or C1-6 alkyl, R = (1-3-Me-substituted) C2-12 alkylene, (1-3-Me-substituted) C $\leq$ 12 cycloalkylene] at 0.5 mol I/NCO equiv and optionally with monoamines and(or) alcs. at NCO:OH/NH 1:0.1-0.3 in an inert solvent.

IT 208587-38-6P, reaction products with dibutylamine

208587-38-6P 208594-47-2DP, reaction products with butanol 208594-49-4P 208666-50-6P

(polyaddn. compds. of uretdione group-containing diisocyanate dimers and amino alcs. for crosslinkers for polyurethane powders)

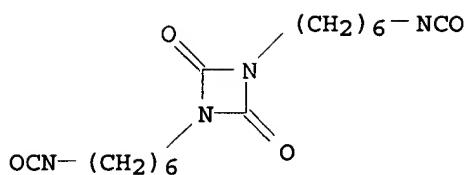
RN 208587-38-6 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatoethyl)-, polymer with 2-aminoethanol (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

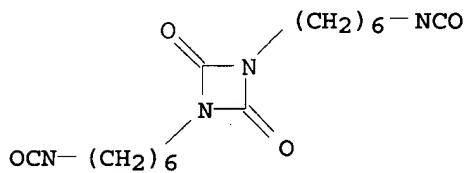
CMF C16 H24 N4 O4



CM 2

CRN 141-43-5  
CMF C2 H7 N OH<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-OHRN 208587-38-6 HCPLUS  
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer  
with 2-aminoethanol (9CI) (CA INDEX NAME)

CM 1

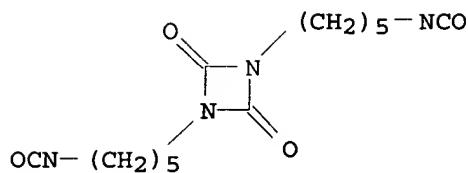
CRN 23501-81-7  
CMF C16 H24 N4 O4

CM 2

CRN 141-43-5  
CMF C2 H7 N OH<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-OHRN 208594-47-2 HCPLUS  
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(5-isocyanatomethylpentyl)-,  
polymer with 2-(methylamino)ethanol (9CI) (CA INDEX NAME)

CM 1

CRN 208594-46-1  
CMF C16 H24 N4 O4  
CCI IDS

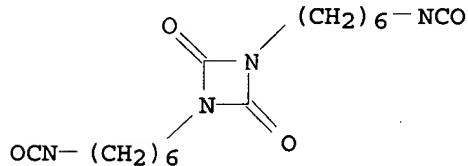


2 ( D1-Me )

CM 2

CRN 109-83-1  
CMF C3 H9 N OHO-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>3</sub>RN 208594-49-4 HCPLUS  
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanato-2-methylhexyl)-, polymer with 2-aminoethanol (9CI) (CA INDEX NAME)

CM 1

CRN 208594-48-3  
CMF C22 H36 N4 O4  
CCI .IDS

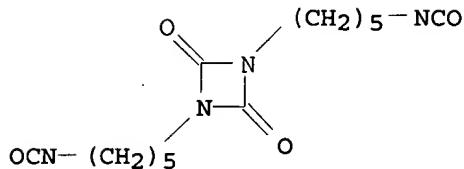
6 ( D1-Me )

CM 2

CRN 141-43-5  
CMF C2 H7 N OH<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-OHRN 208666-50-6 HCPLUS  
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(5-isocyanato-2(or 4)-methylpentyl)-, polymer with 1-amino-2-propanol (9CI) (CA INDEX NAME)

CM 1

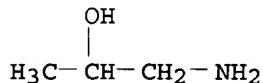
CRN 208594-46-1  
 CMF C16 H24 N4 O4  
 CCI IDS



2 (D1-Me)

CM 2

CRN 78-96-6  
 CMF C3 H9 N O



IC ICM C08G018-79  
 ICS C08G018-32; C09D175-04; C09D005-46; C08L075-04  
 CC 37-6 (Plastics Manufacture and Processing)  
 ST uretdione diisocyanate amino alc polyadduct manuf;  
 polyurethane powder latent crosslinker  
 IT Crosslinking agents  
 (latent; polyaddn. compds. of uretdione group-containing  
 diisocyanate dimers and amino alc. for crosslinkers  
 for polyurethane powders)  
 IT Polyurethanes, uses  
 (polyaddn. compds. of uretdione group-containing  
 diisocyanate dimers and amino alc. for crosslinkers  
 for polyurethane powders)  
 IT Polyurethanes, preparation  
 Polyurethanes, preparation  
 (polyurea-; polyaddn. compds. of uretdione group-containing  
 diisocyanate dimers and amino alc. for crosslinkers  
 for polyurethane powders)  
 IT Polyureas  
 Polyureas  
 (polyurethane-; polyaddn. compds. of uretdione  
 group-containing diisocyanate dimers and amino alc. for  
 crosslinkers for polyurethane powders)  
 IT Alcohols, preparation  
 Amines, preparation  
 (reaction products, with uretdione group-containing  
 diisocyanate-amino alc. copolymers; polyaddn. compds.  
 of uretdione group-containing diisocyanate dimers and

amino alcs. for crosslinkers for polyurethane powders)

IT 71-36-3DP, 1-Butanol, reaction products with uretdione group-containing diisocyanate dimer-amino alcs. copolymers, preparation 111-92-2DP, Dibutylamine, reaction products with uretdione group-containing diisocyanate dimer-amino alcs. copolymers 208587-38-6DP, reaction products with dibutylamine 208587-38-6P 208587-39-7DP, reaction products with dibutylamine 208587-39-7P 208594-47-2DP, reaction products with butanol 208594-49-4P 208666-50-6P  
(polyaddn. compds. of uretdione group-containing diisocyanate dimers and amino alcs. for crosslinkers for polyurethane powders)

L50 ANSWER 10 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:15965 HCAPLUS

DOCUMENT NUMBER: 128:89733

TITLE: Microcapsules with walls from conversion products of uretdione group-containing polyisocyanates and guanidine derivatives

INVENTOR(S): Hagedorn, Manfred; Nehen, Ulrich; Ramzy, Sabry; Klug, Guenter; Weisser, Juergen

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Ger. Offen., 10 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

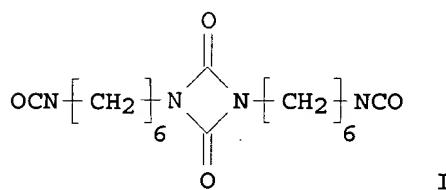
PATENT INFORMATION:

| PATENT NO.  | KIND  | DATE     | APPLICATION NO.  | DATE  |
|-------------|-------|----------|------------------|-------|
| -----       | ----  | -----    | -----            | ----- |
| -----       | ----- | -----    | -----            | ----- |
| DE 19623566 | A1    | 19971218 | DE 1996-19623566 | 1996  |

PRIORITY APPLN. INFO.: DE 1996-19623566

0613  
1996  
0613

GI



AB Microcapsules with high d. and good storage stability, useful for carbonless copying paper, have walls prepared by reaction of the title compds. Typical microcapsules were manufactured by mixing a 10% aqueous guanidine carbonate solution with an emulsion containing crystal violet lactone, diisopropylnaphthalene, polyvinyl alc., and a

60:40 diisocyanate I-OCN(CH<sub>2</sub>)<sub>6</sub>NHCON[(CH<sub>2</sub>)<sub>6</sub>NCO]CONH(CH<sub>2</sub>)<sub>6</sub>  
NCO mixture 90 min at 80°.

IT 200507-27-3P

(microcapsules with walls from conversion products of uretdione group-containing polyisocyanates and guanidine derivs. for carbonless copying paper)

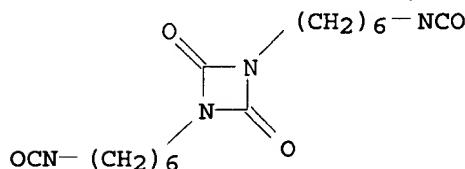
RN 200507-27-3 HCPLUS

CN Carbonic acid, compd. with guanidine (1:2), polymer with 1,3-bis(6-isocyanatohexyl)-1,3-diazetidine-2,4-dione and N,N',2-tris(6-isocyanatohexyl)imidodicarbonic diamide (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

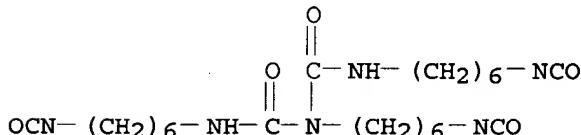
CMF C<sub>16</sub> H<sub>24</sub> N<sub>4</sub> O<sub>4</sub>



CM 2

CRN 4035-89-6

CMF C<sub>23</sub> H<sub>38</sub> N<sub>6</sub> O<sub>5</sub>



CM 3

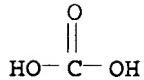
CRN 593-85-1

CMF C H<sub>5</sub> N<sub>3</sub> . 1/2 C H<sub>2</sub> O<sub>3</sub>

CM 4

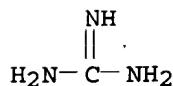
CRN 463-79-6

CMF C H<sub>2</sub> O<sub>3</sub>



CM 5

CRN 113-00-8  
 CMF C H5 N3



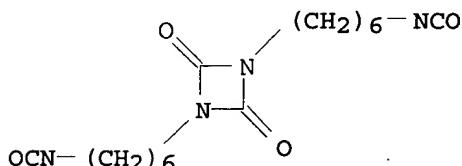
IC ICM B01J013-16  
 ICA B41M005-165  
 CC 38-3 (Plastics Fabrication and Uses)  
 Section cross-reference(s): 74  
 ST microcapsule guanidine uretdione contg polyurea; carbonless  
 copying paper microcapsule polyurea; **hexanediisocyanate**  
 based uretdione contg polyurea microcapsule  
 IT Copying paper  
 Microcapsules  
 (microcapsules with walls from conversion products of uretdione  
 group-containing **polyisocyanates** and guanidine derivs.  
 for carbonless copying paper)  
 IT Polyureas  
 (uretdione-containing; microcapsules with walls from conversion  
 products of uretdione group-containing **polyisocyanates**  
 and guanidine derivs. for carbonless copying paper)  
 IT 200507-27-3P  
 (microcapsules with walls from conversion products of uretdione  
 group-containing **polyisocyanates** and guanidine derivs.  
 for carbonless copying paper)

L50 ANSWER 11 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1997:632095 HCPLUS  
 DOCUMENT NUMBER: 127:248526  
 TITLE: Polyaddition products of dissecondary diamines  
 and **polyisocyanate** mixtures  
 containing uretdione groups  
 INVENTOR(S): Wolf, Elmar  
 PATENT ASSIGNEE(S): Huels Aktiengesellschaft, Germany  
 SOURCE: Eur. Pat. Appl., 7 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.   | KIND | DATE     | APPLICATION NO.  | DATE         |
|--|------|----------|------------------|--------------|
| EP 795569  | A1   | 19970917 | EP 1997-100842   | 1997<br>0121 |
| R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE<br>DE 19610465 | A1   | 19970918 | DE 1996-19610465 | 1996<br>0316 |
| JP 10036483  | A2   | 19980210 | JP 1997-58184    | 1997<br>0313 |
| CA 2200044   | AA   | 19970916 | CA 1997-2200044  | 1997         |

|                    |   |          |                |      |
|--------------------|---|----------|----------------|------|
| US 5912314         | A | 19990615 | US 1997-819365 | 0314 |
| 1997               |   |          |                |      |
| 0317               |   |          |                |      |
| RITY APPLN. INFO.: |   |          |                |      |
| DE 1996-19610465   |   |          |                | A    |
| 1996               |   |          |                |      |
| 0316               |   |          |                |      |

|    |   |
|----|---|
| AB | The title products, useful as curing agents for polyurethanes (e.g., powder coatings) (no data), are prepared from uretdione derivative polyisocyanates [ $\geq 40$ mol% IPDI uretdione diisocyanate] and disecondary diamines (NCO-NH ratio 1:0.5-0.9) at room temp .-60° in inert solvents. Reaction of 3 equivalent N,N'-bis[3-methyl-1-(3-methylpropyl)butyl]-2,2 (or 4),4-trimethyl-1,6-hexanediamine (prepared in >98% purity by reductive amination of the diprimary diamine with iso-Bu <sub>2</sub> CO) with 4 equivalent 1:1 mixture of HMDI and IPDI uretdione derivative diisocyanates gave a product with m.p. 68-81° and NCO content 2.6 and 12.5% before and after, resp., being heated at 180°. |
| IT | 23501-81-7DP, 1,3-Bis(6-isocyanatohexyl)-2,4-uretdione, reaction products with disecondary diamines (polyaddn. products of disecondary diamines and polyisocyanate mixts. containing uretdione groups)  |
| RN | 23501-81-7 HCPLUS   |
| CN | 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)  |



IC ICM C08G018-79  
ICS C08G018-32; C08G018-80  
CC 35-2 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 27  
ST diamine disecondary adduct **diisocyanate**; uretdione  
**diisocyanate** adduct diamine; HMDI uretdione adduct  
diamine; IPDI uretdione adduct diamine; crosslinker  
**polyurethane** powder coating  
IT Crosslinking agents  
(adducts of disecondary diamines and uretdione  
**diisocyanates** as crosslinking agents for  
**polyurethane** powder coatings)  
IT Polyurethanes, uses  
(adducts of disecondary diamines and uretdione  
**diisocyanates** as crosslinking agents for  
**polyurethane** powder coatings)  
IT Amines, preparation  
(diamines, disecondary, reaction products with uretdione  
**diisocyanates**; polyaddn. products of disecondary  
diamines and **polyisocyanate** mixts. containing uretdione  
groups)  
IT Coating materials

(powder; adducts of dissecondary diamines and uretdione diisocyanates as crosslinking agents for polyurethane powder coatings)

IT 192528-25-9DP, reaction products with uretdione diisocyanates  
(polyaddn. products of dissecondary diamines and polyisocyanate mixts. containing uretdione groups)

IT 23501-81-7DP, 1,3-Bis(6-isocyanatoethyl)-2,4-uretdione, reaction products with dissecondary diamines 41094-42-2DP, N,N'-Diisobutylisophoronediamine, reaction products with uretdione diisocyanates 53895-31-1DP, IPDI dimer, uretdione group-containing, reaction products with dissecondary diamines 192462-35-4DP, reaction products with uretdione diisocyanates 192528-26-0DP, reaction products with uretdione diisocyanates  
(polyaddn. products of dissecondary diamines and polyisocyanate mixts. containing uretdione groups)

L50 ANSWER 12 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:513130 HCAPLUS

DOCUMENT NUMBER: 125:144831

TITLE: One component-type fast heat-curable polyurethane elastomer compositions and their molding method

INVENTOR(S): Hirayama, Shinji; Konishi, Shin; Hashimoto, Sadako; Morikawa, Yukihiro

PATENT ASSIGNEE(S): Inoue MTP KK, Japan; Nippon Polyurethane Kogyo KK; Nippon Polyurethane Industry Co., Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE         |
|------------------------|------|----------|-----------------|--------------|
| JP 08134164            | A2   | 19960528 | JP 1994-306908  | 1994<br>1115 |
| JP 3509967             | B2   | 20040322 | JP 1994-306908  | 1994<br>1115 |
| PRIORITY APPLN. INFO.: |      |          |                 |              |

AB The title compns. comprise (1) polyurethane precursors with equivalent ratio of uretdione group to active H (r-1) 0.25-1.0 prepared by treating (A) polyisocyanates at least containing polyisocyanates with uretdione groups and (B) ≥2 active H-containing compds. with mol. weight 18-20,000 at equivalent ratio of the active H to the NCO (r-2) >1.0 and (2) 1,5-diazabicyclo[4.3.0]nonene-5 (DBN) and/or their salts. The title molding method comprises injecting the compns. at a temperature lower or equal to the ring-opening temperature of the uretdione group (T), molding, and heating at a temperature higher or equal to T for reacting and curing. Thus, 100 parts a composition comprising a precursor with r-1 0.72 prepared by treating uretdione group-containing HDI derivative and polytetramethylene ether polyol at ratio r-2 1.3, 0.5 part DBN, and 0.5 part Irganox 1010 were fed to a reactor and stirred at 80° to give a composition, which was

press molded and cured at 200°.

IT 180163-58-0P

(rubber; one component-type fast heat-curable polyurethane elastomer compns. and their molding method)

RN 180163-58-0 HCPLUS

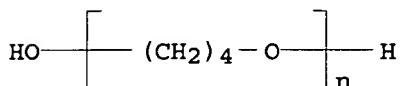
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatoethyl)-, polymer with  $\alpha$ -hydro- $\omega$ -hydroxypoly(oxy-1,4-butanediyl) (9CI)  
(CA INDEX NAME)

CM 1

CRN 25190-06-1

CMF (C<sub>4</sub> H<sub>8</sub> O)<sub>n</sub> H<sub>2</sub> O

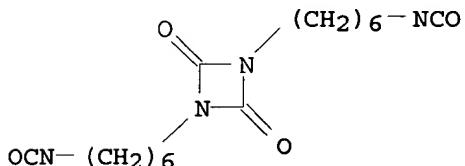
CCI PMS



CM 2

CRN 23501-81-7

CMF C<sub>16</sub> H<sub>24</sub> N<sub>4</sub> O<sub>4</sub>



IC ICM C08G018-10

ICS C08G018-20; C08G018-70; C08G018-79

CC 39-9 (Synthetic Elastomers and Natural Rubber)

IT 180163-58-0P

(rubber; one component-type fast heat-curable polyurethane elastomer compns. and their molding method)

L50 ANSWER 13 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:209693 HCPLUS

DOCUMENT NUMBER: 124:235011

TITLE: Liquid polyisocyanates containing aromatic and aliphatic isocyanate groups for use in lacquers

INVENTOR(S): Brahm, Martin; Pedain, Josef; Schmalstieg, Lutz

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Eur. Pat. Appl., 8 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

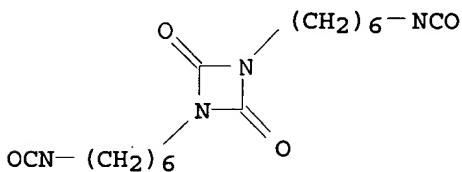
|                                   |    |          |                 |                   |
|-----------------------------------|----|----------|-----------------|-------------------|
| EP 696606                         | A1 | 19960214 | EP 1995-111814  | 1995<br>0727      |
| EP 696606                         | B1 | 19991124 |                 |                   |
| R: AT, BE, DE, ES, FR, GB, IT, NL |    |          |                 |                   |
| DE 4428107                        | A1 | 19960215 | DE 1994-4428107 | 1994<br>0809      |
| AT 186928                         | E  | 19991215 | AT 1995-111814  | 1995<br>0727      |
| ES 2139791                        | T3 | 20000216 | ES 1995-111814  | 1995<br>0727      |
| US 5606004                        | A  | 19970225 | US 1995-509258  | 1995<br>0727      |
| CA 2155473                        | AA | 19960210 | CA 1995-2155473 | 1995<br>0731      |
| JP 08059771                       | A2 | 19960305 | JP 1995-219446  | 1995<br>0804      |
| JP 3604204                        | B2 | 20041222 |                 | 1995<br>0807      |
| PRIORITY APPLN. INFO.:            |    |          | DE 1994-4428107 | A<br>1994<br>0809 |

AB The title **polyisocyanates** are prepared by mixed trimerization of TDI (optionally containing other aromatic isocyanates) with aliphatic **isocyanates** (e.g., uretedione group-containing dimer of HDI). The **polyisocyanates** are especially useful as crosslinkers for OH-containing binders in two-component **polyurethane** lacquers.

IT 23501-81-7DP, 1,3-Bis(6-isocyanatohexyl)  
)-1,3-diazetidine-2,4-dione, reaction products with TDI  
(liquid; preparation and use as crosslinkers for two-component  
polyurethane lacquers)

RN 23501-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl) - (9CI) (CA INDEX NAME)



IC ICM C08G018-79  
ICS C08G018-02

CC 42-10 (Coatings, Inks, and Related Products)

ST liq aliph arom polyisocyanate crosslinker  
polyurethane; TDI HDI polyisocyanate liq  
crosslinker polyurethane; lacquer polyurethane

IT crosslinker liq polyisocyanate  
 Coating materials  
 (liquid polyisocyanates prepared from aromatic and aliphatic isocyanates for use as hardeners in two-component polyurethane lacquers)

IT Urethane polymers, uses  
 (liquid polyisocyanates prepared from aromatic and aliphatic isocyanates for use as hardeners in two-component polyurethane lacquers)

IT Crosslinking agents  
 (liquid polyisocyanates prepared from aromatic and aliphatic isocyanates for use in two-component polyurethane lacquers)

IT 584-84-9DP, 2,4-Tdi, reaction products with aliphatic polyisocyanates 26471-62-5DP, TDI, reaction products with aliphatic polyisocyanates  
 (liquid; preparation and use as crosslinkers for two-component polyurethane lacquers)

IT 23501-81-7DP, 1,3-Bis(6-isocyanatohexyl)  
 )-1,3-diazetidine-2,4-dione, reaction products with TDI  
 28574-90-5DP, Hexamethylene diisocyanate trimer,  
 reaction products with TDI  
 (liquid; preparation and use as crosslinkers for two-component polyurethane lacquers)

L50 ANSWER 14 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:130831 HCAPLUS

DOCUMENT NUMBER: 124:205122

TITLE: Coating compositions containing aldimines and isocyanates

INVENTOR(S): Braun, David W.; Colyer, Emmerson Keith;  
 Dantiki, Sudhakar; Tye, Anthony J.; Shah, Rajnikant P.; Mormile, Patrick J.; Richards, Bradley M.; Koevenig, Brian P.; Laginess, Thomas J.; Stateczny, Henry J.

PATENT ASSIGNEE(S): BASF Corp., USA

SOURCE: Eur. Pat. Appl., 27 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE         |
|---|------|----------|-----------------|--------------|
| EP 686654   | A1   | 19951213 | EP 1995-107978  | 1995<br>0526 |
| EP 686654   | B1   | 20031001 |                 |              |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE |      |          |                 |              |
| AT 251190   | E    | 20031015 | AT 1995-107978  | 1995<br>0526 |
| ES 2208660  | T3   | 20040616 | ES 1995-107978  | 1995<br>0526 |
| AU 9520459  | A1   | 19951214 | AU 1995-20459   | 1995<br>0602 |

|                        |    |          |                 |    |      |
|------------------------|----|----------|-----------------|----|------|
| AU 701598              | B2 | 19990204 |                 |    |      |
| CA 2151014             | AA | 19951207 | CA 1995-2151014 |    | 1995 |
|                        |    |          |                 |    | 0605 |
| BR 9502671             | A  | 19970805 | BR 1995-2671    |    | 1995 |
|                        |    |          |                 |    | 0605 |
| JP 08060089            | A2 | 19960305 | JP 1995-162929  |    | 1995 |
|                        |    |          |                 |    | 0606 |
| ZA 9504597             | A  | 19961205 | ZA 1995-4597    |    | 1996 |
|                        |    |          |                 |    | 0605 |
| AU 9888361             | A1 | 19981203 | AU 1998-88361   |    | 1998 |
|                        |    |          |                 |    | 1008 |
| AU 736624              | B2 | 20010802 | US 1994-254211  | A  | 1994 |
| PRIORITY APPLN. INFO.: |    |          |                 |    | 0606 |
|                        |    |          | AU 1995-20459   | A3 | 1995 |
|                        |    |          |                 |    | 0602 |

AB High-solids compns. with good pot life for coatings contain (a) (R1CH:N)nR2 [R1 = (substituted) alkyl, (substituted) aryl, (substituted) cycloalkyl, substituted heterocyclic group, R2 = monomeric or polymeric aliphatic, aromatic, arylaliph. or cycloaliph. group which may contain O, N, S, or Si, n > 1], (b) a polyisocyanate functional component, and (c) optionally, other active hydrogen compds. A typical composition contained 1:2 (mol ratio) isophoronediamine-isobutyraldehyde adduct 72.56, catalyst 0.82, HDI uretdione 90.88, and flow modifier and photostabilizers 5.75 parts.

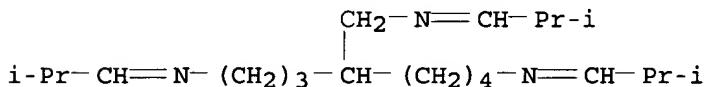
IT 173923-56-3P 174423-54-2P  
(high-solids compns. containing aldimines and polyisocyanates with good pot life for coatings)

RN 173923-56-3 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatoethyl)-, polymer with N,N'-bis(2-methylpropylidene)-4-[[[(2-methylpropylidene)amino]methyl]-1,8-octanediamine (9CI) (CA INDEX NAME)

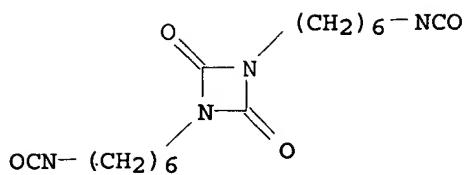
CM 1

CRN 173923-55-2  
CMF C21 H41 N3



CM 2

CRN 23501-81-7  
CMF C16 H24 N4 O4



RN 174423-54-2 HCPLUS

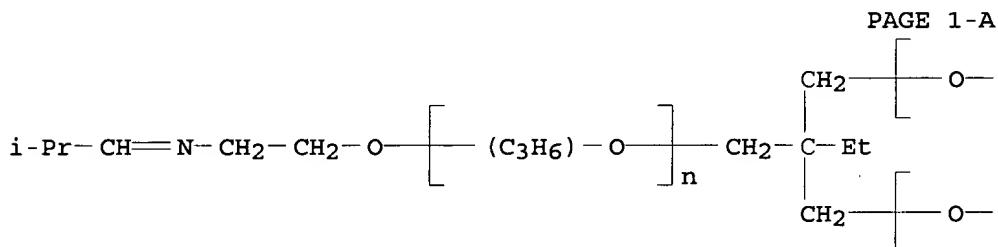
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with  $\alpha$ -hydro- $\omega$ -[methyl-2-[(2-methylpropylidene)amino]ethoxy]poly[oxy(methyl-1,2-ethanediyl)]ether with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (3:1) (9CI) (CA INDEX NAME)

CM 1

CRN 174423-53-1

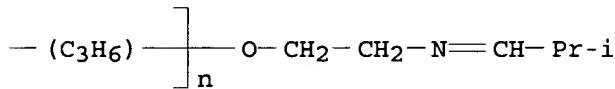
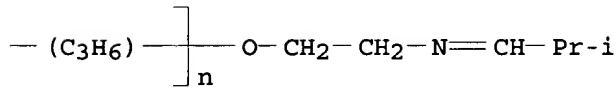
CMF (C<sub>3</sub> H<sub>6</sub> O)<sub>n</sub> (C<sub>3</sub> H<sub>6</sub> O)<sub>n</sub> (C<sub>3</sub> H<sub>6</sub> O)<sub>n</sub> C<sub>27</sub> H<sub>53</sub> N<sub>3</sub> O<sub>3</sub>

CCI IDS, PMS



3 ( D1-Me )

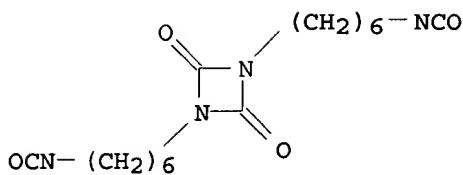
PAGE 1-B



CM 2

CRN 23501-81-7

CMF C<sub>16</sub> H<sub>24</sub> N<sub>4</sub> O<sub>4</sub>



IC ICM C08G018-32  
 ICS C08G018-79; C09D017-00; C09D007-02; C07C251-16  
 CC 42-10 (Coatings, Inks, and Related Products)  
 ST polyisocyanate aldimine copolymer coating; storage  
 stable polyisocyanate aldimine coating; isophorone  
 bisisobutyldimine HDI uretdione copolymer coating  
 IT Polyamides, uses  
     (imine-group-containing; high-solids compns. containing aldimines and  
     polyisocyanates with good pot life for coatings)  
 IT Coating materials  
     (high-solids, high-solids compns. containing aldimines and  
     polyisocyanates with good pot life for coatings)  
 IT Polyisocyanurates  
     (polyamide-, imine- and uretdione-group-containing; high-solids  
     compns. containing aldimines and polyisocyanates with  
     good pot life for coatings)  
 IT Polyamides, uses  
     (polyisocyanurate-, imine- and uretdione-group-containing;  
     high-solids compns. containing aldimines and  
     polyisocyanates with good pot life for coatings)  
 IT 173923-54-1P 173923-56-3P 173923-58-5P 173923-60-9P  
     173923-61-0P 173923-62-1P 174423-54-2P 174587-94-1P  
     (high-solids compns. containing aldimines and  
     polyisocyanates with good pot life for coatings)

L50 ANSWER 15 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1994:633093 HCAPLUS  
 DOCUMENT NUMBER: 121:233093  
 TITLE: New aliphatic polyisocyanate curing agents for  
       higher solids urethane coatings  
 AUTHOR(S): Wojcik, R. T.; Goldstein, S. L.; Malofsky, A.  
       G.; Barnowski, H. G., Jr.; Chandalia, K. B.  
 CORPORATE SOURCE: Chem. Res. Cent., Olin Corp., Cheshire, CT,  
       06410, USA  
 SOURCE: Proceedings of the Waterborne, High-Solids,  
       and Powder Coatings Symposium (1993), 20th,  
       26-48  
 CODEN: PWHSE6  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Polyisocyanate curing agents prepared from hexamethylene  
       diisocyanate (HDI) are used com. in High Solids Paints for  
       automotive, maintenance, and industrial finishes. These products  
       are based on isocyanurate or biuret chemical. Olin has an active  
       research program to develop low viscosity polyisocyanates. In  
       this program, the authors made very pure HDI isocyanurate trimer  
       and HDI uretdione cross-linkers and studied their effect on 2K  
       polyurethane coatings processing and performance. These curing  
       agents were formulated into High Solids Paints with com. available  
       polyols. Appearance VOC, paint coverage, coating appearance  
       (gloss & DOI), mech. performance (hardness, flexibility, and

impact), environmental durability (gloss retention, chalking, and cracking), and chemical/moisture resistance were compared to standard 2K polyurethane coatings formulated with com. HDI polyisocyanurate (Luxate<sup>TM</sup> HT2000). The coatings made with the new curing agent had lower VOC and superior appearance compared to the com. polyisocyanate. The mech. properties and environmental durability of the coatings were similar. Compared to the coatings made with Luxate<sup>TM</sup> HT2000, these curing agents had slower dry times and reduced surface hardness. This paper suggests formulation methods to decrease the dry times and increase surface hardness.

IT 158407-53-5 158407-54-6

(New aliphatic polyisocyanate curing agents for higher solids urethane coatings)

RN 158407-53-5 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with G-Cure 105P70 (9CI) (CA INDEX NAME)

CM 1

CRN 158191-40-3

CMF Unspecified

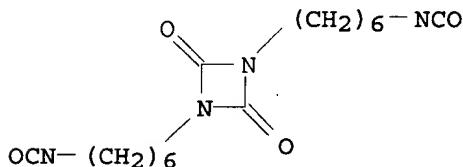
CCI PMS, MAN

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

CM 2

CRN 23501-81-7

CMF C16 H24 N4 O4



RN 158407-54-6 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with Acryloid AU 946 and QM 1007 (9CI) (CA INDEX NAME)

CM 1

CRN 158191-13-0

CMF Unspecified

CCI PMS, MAN

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

CM 2

CRN 115628-82-5

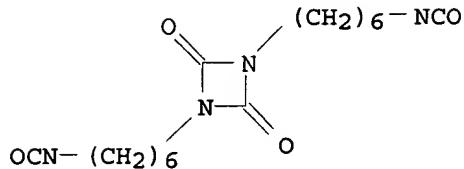
CMF Unspecified

CCI PMS, MAN

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

CM 3

CRN 23501-81-7  
CMF C16 H24 N4 O4

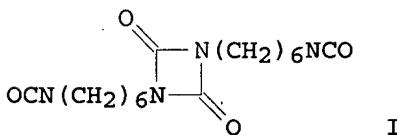


CC 42-3 (Coatings, Inks, and Related Products)  
IT 158407-53-5 158407-54-6  
(New aliphatic polyisocyanate curing agents for higher solids urethane coatings)

L50 ANSWER 16 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1994:484214 HCAPLUS  
DOCUMENT NUMBER: 121:84214  
TITLE: Process for producing uretidione dimers of isocyanates using catalysts which are bound to inorganic matrixes  
INVENTOR(S): Goldstein, Stephen L.; Hamer, Anthony D.; Katz, Lawrence E.; McGahey, Michael J.; Smith, Curtis P.  
PATENT ASSIGNEE(S): Olin Corp., USA  
SOURCE: U.S., 7 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE               |
|------------------------|------|----------|-----------------|--------------------|
| US 5315004             | A    | 19940524 | US 1993-43075   | 1993<br>0405       |
| US 5461020             | A    | 19951024 | US 1994-241249  | 1994<br>0511       |
| PRIORITY APPLN. INFO.: |      |          | US 1993-43075   | A2<br>1993<br>0405 |

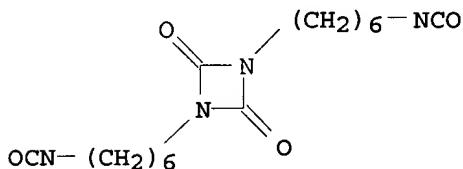
GI



AB The invention relates to a process for preparing a dimer by

cyclodimerizing a polyisocyanate in the presence of a dimerization catalyst which is covalently bound to an insol. inorg. matrix. Said polyisocyanate is contacted with the catalyst at a temperature of between 20-135°C to form an uretidione (cyclodimerized isocyanate). Thus, silica-bound N,N-bis[3-(diethoxymethylsilyl)propyl]-4-pyridinamine was used as cyclodimerization catalyst for HDI. The IR spectrum of the products showed no absorption due to isocyanurates; 15% of HDI were converted to hexamethylene diisocyanate dimer [1,3-bis(6-isocyanatohexyl)-2,4-uretidinedione] (I).

IT 23501-81-7P, Hexamethylene diisocyanate dimer  
(preparation of, with inorg. matrix-bound (dialkylamino)pyridine as  
cyclodimerization catalyst)  
RN 23501-81-7 HCPLUS  
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl) - (9CI) (CA  
INDEX NAME)



IC ICM C07D229-00  
ICS C08G018-74  
INCL 540202000  
CC 35-2 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 27, 28  
ST uretidione hexamethylene **diisocyanate** dimer;  
cyclodimerization catalyst pyridinamine silica bound  
IT Glass, nonoxide  
    (cyclodimerization catalyst-supports for **diisocyanate**  
    )  
IT Clays, uses  
Zeolites, uses  
    (inorg. matrix-bound amines as cyclodimerization catalysts for  
    **diisocyanates**)  
IT Glass, oxide  
    (inorg. matrix-bound, cyclodimerization catalysts for  
    **diisocyanate**)  
IT Amines, uses  
    (aryl, inorg. matrix-bound, cyclodimerization catalysts for  
    **diisocyanate**)  
IT Dimerization catalysts  
    (cyclo-, inorg. matrix-bound (dialkylamino)pyridine for  
    **isocyanates**)  
IT Dimerization  
    (cyclo-, of **diisocyanates** with inorg. matrix-bound  
    (dialkylamino)pyridine)  
IT Amines, uses  
    (tertiary, inorg. matrix-bound, cyclodimerization catalysts for  
    **diisocyanate**)  
IT 128823-47-2D, 4-Pyridinamine, N,N-bis[3-  
(diethoxymethylsilyl)propyl]-, inorg. matrix-bound 129677-07-2D,  
4-Pyridinamine, N-[(ethenylphenyl)methyl]-N-methyl-, inorg.  
matrix-bound  
    (as cyclodimerization catalyst for **diisocyanate**)

IT 1344-28-1, Aluminum oxide (Al<sub>2</sub>O<sub>3</sub>), uses 7631-86-9, Silica, uses (inorg. matrix-bound amines as cyclodimerization catalysts for diisocyanates)

IT 7803-51-2D, Phosphine, alkyl or alkylamino derivs. (inorg. matrix-bound, cyclodimerization catalysts for diisocyanate)

IT 23501-81-7P, Hexamethylene diisocyanate dimer  
26747-90-0P, TDI dimer 53895-31-1P, IPDI dimer (preparation of, with inorg. matrix-bound (dialkylamino)pyridine as cyclodimerization catalyst)

L50 ANSWER 17 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:247474 HCAPLUS

DOCUMENT NUMBER: 120:247474

TITLE: Use of alkylthio-substituted aromatic diamines as curing agents for polyisocyanates in coating and sealing compositions

INVENTOR(S): Hentschel, Karl Heinz; Walter, Ulrich

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

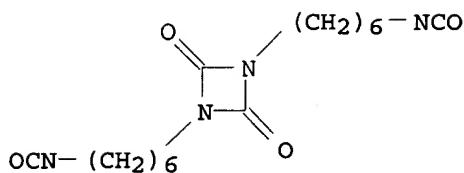
| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE              |
|------------------------|------|----------|-----------------|-------------------|
| EP 570798              | A1   | 19931124 | EP 1993-107559  | 1993<br>0510      |
| DE 4217023             | A1   | 19931125 | DE 1992-4217023 | 1992<br>0522      |
| CA 2096466             | AA   | 19931123 | CA 1993-2096466 | 1993<br>0518      |
| JP 06049410            | A2   | 19940222 | JP 1993-139886  | 1993<br>0520      |
| PRIORITY APPLN. INFO.: |      |          | DE 1992-4217023 | A<br>1992<br>0522 |

AB Arom diamines containing  $\geq 1$  C1-4 alkylthio group ortho to each amino group, especially a mixture of 2,4- and 2,6-diamino-1-methyl-3,5-bis(methylthio)benzenes, are used, optionally with other polyamines and/or polyols, as hardeners for polyisocyanates in 2-component coating or sealing compns. which contain little or no solvent and cure at room temp. without forming bubbles or voids.

IT 23501-81-7DP, Hexamethylene diisocyanate dimer, polymers with alkylthio aromatic diamines and polyols (preparation of, for two-component coating and sealing compns.)

RN 23501-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



IC ICM C08G018-38  
 ICS C08G018-10; C09D175-02; C04B041-48; C09K003-10  
 CC 42-10 (Coatings, Inks, and Related Products)  
 ST amine arom alkylthio polyurea **polyurethane**; sulfide  
 amine arom polyurea **polyurethane**; crosslinking alkylthio  
 amine polyurea **polyurethane**; sealant polyurea  
**polyurethane** alkylthio amine  
 IT Crosslinking agents  
 (diamines, aromatic, alkylthio, for **polyurea-polyurethanes**  
 in coatings and sealants)  
 IT **Urethane polymers, preparation**  
 (polyurea-, preparation of, for two-component coatings and sealants,  
 alkylthio aromatic diamines in)  
 IT Coating materials  
 Sealing compositions  
 (two-component, **polyurea-polyurethanes** for, alkylthio  
 aromatic diamine-containing)  
 IT 584-84-9DP, 2,4-Diisocyanatotoluene, polymers with  
 alkylthio aromatic diamines, and polyols 822-06-0DP, HDI, polymers  
 with alkylthio aromatic diamines and polyols 3779-63-3DP, polymers  
 with alkylthio aromatic diamines and polyols 5873-54-1DP, 2,4'-  
**Diisocyanatodiphenylmethane**, polymers with alkylthio aromatic  
 diamines and polyols 9016-87-9DP, PAPI, polymers with alkylthio  
 aromatic diamines and polyols 23501-81-7DP, Hexamethylene  
**diisocyanate** dimer, polymers with alkylthio aromatic diamines  
 and polyols 25322-69-4DP, Polypropylene glycol, polymers with  
 alkylthio aromatic diamines and **polyisocyanates**  
 25723-16-4DP, Polypropylene glycol trimethylolpropane ether,  
 polymers with alkylthio aromatic diamines and **polyisocyanates**  
 26471-62-5DP, Tdi, polymers with alkylthio aromatic diamines and  
 polyols 54511-70-5DP, polymers with alkylthio aromatic diamines and  
**polyisocyanates** 102093-68-5DP, polymers with  
**polyisocyanates** and polyols 104983-85-9DP, polymers with  
**polyisocyanates** and polyols 106264-79-3DP, Ethacure 300,  
 polymers with **polyisocyanates** and polyols  
 107120-02-5DP, polymers with alkylthio aromatic diamines and  
**polyisocyanates**  
 (preparation of, for two-component coating and sealing compns.)

L50 ANSWER 18 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:137262 HCPLUS  
 DOCUMENT NUMBER: 120:137262  
 TITLE: Aqueous **polyurethane** binder  
 combination, process for its preparation and  
 its use  
 INVENTOR(S): Blum, Harald; Kubitza, Werner; Probst,  
 Joachim; Sonntag, Michael; Schneider, Volker  
 PATENT ASSIGNEE(S): Bayer A.-G., Germany  
 SOURCE: Eur. Pat. Appl., 20 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent

LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.   | KIND     | DATE                 | APPLICATION NO. | DATE              |
|--|----------|----------------------|-----------------|-------------------|
| EP 542105  | A1       | 19930519             | EP 1992-118831  | 1992<br>1103      |
| EP 542105<br>R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE<br>DE 4137429 | B1<br>A1 | 19960124<br>19930519 | DE 1991-4137429 | 1991<br>1114      |
| AT 133430  | E        | 19960215             | AT 1992-118831  | 1992<br>1103      |
| ES 2084909   | T3       | 19960516             | ES 1992-118831  | 1992<br>1103      |
| US 5331039   | A        | 19940719             | US 1992-973368  | 1992<br>1109      |
| CA 2082785   | AA       | 19930615             | CA 1992-2082785 | 1992<br>1112      |
| JP 05295072  | A2       | 19931109             | JP 1992-326290  | 1992<br>1112      |
| JP 2923718<br>KR 217448  | B2<br>B1 | 19990726<br>19990901 | KR 1992-21281   | 1992<br>1113      |
| PRIORITY APPLN. INFO.:   |          |                      | DE 1991-4137429 | A<br>1991<br>1114 |

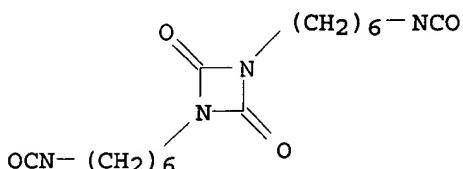
AB The title binders, useful for varnishes, coats, sealants, and adhesives with reduced organic solvent content, are obtained by mixing a **polyisocyanate** component and a H<sub>2</sub>O-thinned polyester-polyol component which is a blend of ≥2 hydroxy-, **urethane**-, carboxy-, or sulfonate-containing (acrylate-grafted) polyester resins. An aqueous dispersion (A) of a polyester-**urethane**-polyol prepared from trimethylolpropane, isophthalic acid, saturated fatty acids (Prifrac 2950), neopentyl glycol, hexahydrophthalic anhydride, dimethylolpropionic acid, and isophorone **diisocyanate** had solids content 48.5%, pH 7.4 (NH<sub>4</sub>OH), acid number 10, and OH group content 4.6%. Another aqueous dispersion (B) prepared by polymerization of 2-hydroxyethyl methacrylate, Me methacrylate, Bu acrylate, and acrylic acid in BuOAc solvent followed by emulsification of the polymer solution in H<sub>2</sub>O with azeotropic removal of the solvent, had solids content 30%, pH 7.0 (NH<sub>4</sub>OH), carboxy group content 139 mequiv/100 g solids, and OH group content 4.6%. A (storage-stable) blend containing A 50, B 50, thickener 1.14, emulsifier 0.8, defoamer 0.93, and deionized H<sub>2</sub>O 4.9 parts was mixed with 28.88 parts solvent-free 70:30 HMDI dimer-HMDI trimer mixture (average NCO group content 22.5%, viscosity 200 mPa·s, 23°) to give a 2-component title binder having NCO/OH ratio

1.5 and open time .apprx.5 h. A 200- $\mu$ m (wet thickness) clear coat was dust-free dry after 2-3 h at room temperature and after 10-14 days had pendulum hardness 100-120 s.

IT 23501-81-7DP, Hexamethylene diisocyanate dimer, polymers with polyester polyols (preparation of aqueous dispersions of, as binders)

RN 23501-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



IC ICM C08G018-42

ICS C08G018-40; C08G018-72; C08G018-08; C09D175-06

CC 42-10 (Coatings, Inks, and Related Products)

Section cross-reference(s): 37

ST polyester aq dispersion prepn **polyurethane binder**; lacquer **polyurethane** aq polyester dispersion; HMDI dimer trimer aq **polyurethane binder**

IT Binding materials

(aqueous **polyurethane** compns.)

IT Sealing compositions

(aqueous **polyurethane** compns. as)

IT Coating materials

(aqueous **polyurethane** compns. for)

IT Adhesives

(binders for, aqueous **polyurethane** compns. as)

IT Fatty acids, compounds

(C14-16, reaction products, with polyols and isophorone **isocyanate**, preparation of, for aqueous **polyurethane** binder compns.)

IT Polyesters, preparation

(sulfo-containing, preparation of aqueous dispersions of, for **polyurethane** binder compns.)

IT Polyesters, preparation

(sulfo-containing, graft, preparation of aqueous dispersions of, for **polyurethane** binder compns.)

IT Polyesters, preparation

(urethane group-containing, preparation of aqueous dispersions of, for **polyurethane** binder compns.)

IT 77-99-6DP, polyester **urethane** polyols, polymers with

**polyisocyanates** 85-42-7DP, Hexahydrophthalic anhydride,

polyester **urethane** polyols, polymers with

**polyisocyanates** 121-91-5DP, 1,3-Benzenedicarboxylic

acid, polyester **urethane** polyols, polymers with

**polyisocyanates** 126-30-7DP, Neopentyl glycol, polyester

**urethane** polyols, polymers with **polyisocyanates**

4098-71-9DP, polyester **urethane** polyols, polymers with

**polyisocyanates** 4767-03-7DP, polyester **urethane**

polyols, polymers with **polyisocyanates**

23501-81-7DP, Hexamethylene diisocyanate dimer,

polymers with polyester polyols 28574-90-5DP, polymers with

polyester polyols

IT (preparation of aqueous dispersions of, as binders)  
 26351-99-5P, Acrylic acid-Butyl acrylate-2-Hydroxyethyl  
 methacrylate-Methyl methacrylate copolymer 153162-68-6P  
 153354-09-7P 153354-10-0P  
 (preparation of aqueous dispersions of, for polyurethane  
 binders)

L50 ANSWER 19 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1994:32937 HCAPLUS  
 DOCUMENT NUMBER: 120:32937  
 TITLE: Modified polyureas for use in coatings  
 INVENTOR(S): Muenzmay, Thomas; Hassel, Tillmann  
 PATENT ASSIGNEE(S): Bayer A.-G., Germany  
 SOURCE: Ger. Offen., 10 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.   | KIND     | DATE                 | APPLICATION NO.                   | DATE              |
|--|----------|----------------------|-----------------------------------|-------------------|
| DE 4133572   | A1       | 19930415             | DE 1991-4133572                   | 1991<br>1010      |
| EP 538649  | A1       | 19930428             | EP 1992-116542                    | 1992<br>0928      |
| EP 538649<br>R: BE, DE, ES, FR, GB, IT, NL, SE<br>ES 2088067 | B1<br>T3 | 19960612<br>19960801 | DE 1991-4133572<br>ES 1992-116542 | 1992<br>0928      |
| US 5284928   | A        | 19940208             | US 1992-956518                    | 1992<br>1005      |
| CA 2079980   | AA       | 19930411             | CA 1992-2079980                   | 1992<br>1006      |
| CA 2079980<br>JP 06122750                                    | C<br>A2  | 20030211<br>19940506 | JP 1992-290963                    | 1992<br>1006      |
| JP 3107665   | B2       | 20001113             | DE 1991-4133572                   | A<br>1991<br>1010 |
| PRIORITY APPLN. INFO.:                                       |          |                      |                                   |                   |

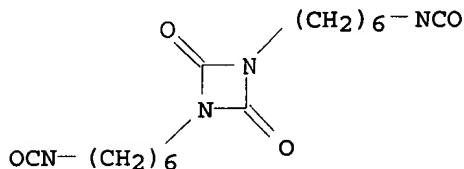
AB Polyureas useful as binders for coatings contain anionic N-[(cyanoamino)carbonyl]urea groups and, optionally, terminal anionic cyanourea groups. Stirring hexanediol polycarbonate (OH number 56) 2240, a monofunctional ethylene oxide-rich polyether (OH number 26) 178, 3,5-bis(6-isocyanatohexyl)tetrahydro-1,3,5-oxadiazine-2,4,6-trione 336.4, HMDI 200.9, and IPDI 442.4 g at 80°, adding 94.8 g 1,4-butanediol, adding 6.5 kg acetone, adding 36.0 g ethylenediamine and 25.0 g hydrazine hydrate in 500 g H<sub>2</sub>O, stirring at 50°, adding a solution of cyanamide 33.6, Et<sub>3</sub>N 80.7, and acetone 300 g, stirring 60 min with removal of CO<sub>2</sub>, adding 8.6 kg H<sub>2</sub>O, and distilling acetone in vacuo

gave a dispersion (31.4% solids) showing DIN cup number 4 viscosity 12.5 s.

IT 23501-81-7DP, polymers with polyols, polyisocyanates and diamines, reaction products with cyanamid, triethylamine salts (coatings, water-thinned, manufacture of)

RN 23501-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



IC ICM C08G018-78

ICS C08G018-79; C08G018-32; C08G018-65; C09D175-02

CC 42-7 (Coatings, Inks, and Related Products)

Section cross-reference(s): 37

ST cyanamid adduct polyurea aq coating; polyurethane polyurea deriv aq coating; cyanobiuret polyurea deriv aq coating; polycarbonate polyurethane aq coating; oxadiazinetrione cyanoethyl copolymer aq coating

IT Urethane polymers, uses

(polycarbonate-polyoxyalkylene-polyurea-, cyanobiuret group-containing, coatings, water-thinned, manufacture of)

IT Polyureas

(polycarbonate-polyoxyalkylene-polyurethane-, cyanobiuret group-containing, coatings, water-thinned, manufacture of)

IT Polyoxyalkylenes, uses

(polycarbonate-polyurea-polyurethane-, cyanobiuret group-containing, coatings, water-thinned, manufacture of)

IT Polycarbonates, uses

(polyoxyalkylene-polyurea-polyurethane-, cyanobiuret group-containing, coatings, water-thinned, manufacture of)

IT 107-15-3DP, 1,2-Ethanediamine, polymers with polyols, polyisocyanates and diamines, reaction products with cyanamid, triethylamine salts 110-63-4DP, 1,4-Butanediol, polymers with polyols, polyisocyanates and diamines, reaction products with cyanamid, triethylamine salts 302-01-2DP, Hydrazine, polymers with polyols, polyisocyanates and diamines, reaction products with cyanamid, triethylamine salts 420-04-2DP, Cyanamide, reaction products with polyureas, triethylamine salts 822-06-0DP, polymers with polyols, polyisocyanates and diamines, reaction products with cyanamid, triethylamine salts 4098-71-9DP, polymers with polyols, polyisocyanates and diamines, reaction products with cyanamid, triethylamine salts 23501-81-7DP, polymers with polyols, polyisocyanates and diamines, reaction products with cyanamid, triethylamine salts 25037-68-7DP, polymers with polyisocyanates, polyols and diamines, reaction products with cyanamide, triethylamine salts 50639-37-7DP, polymers with polyols, polyisocyanates and diamines, reaction products with cyanamid, triethylamine salts 152145-38-5DP, reaction products with cyanamide, triethylamine salts 152145-39-6DP, reaction products with cyanamide,

triethylamine salts  
(coatings, water-thinned, manufacture of)

L50 ANSWER 20 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1994:32124 HCAPLUS  
 DOCUMENT NUMBER: 120:32124  
 TITLE: Free-flowing, thermoplastic, post-curable  
 powdered polyurethanes, optionally expandable  
 INVENTOR(S): Werner, Joachim; Meckel, Walter; Liman,  
 Ulrich; Wegener, Dirk; Rasshofer, Werner;  
 Rosthauser, James W.  
 PATENT ASSIGNEE(S): Bayer A.-G., Germany  
 SOURCE: Eur. Pat. Appl., 18 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

| PATENT NO.                                      | KIND | DATE     | APPLICATION NO. | DATE              |
|---|------|----------|-----------------|-------------------|
| EP 539802                                       | A1   | 19930505 | EP 1992-117604  | 1992<br>1015      |
| R: BE, DE, ES, FR, GB, IT, NL, SE<br>DE 4135475 | A1   | 19930429 | DE 1991-4135475 | 1991<br>1028      |
| DE 4209709                                      | A1   | 19930930 | DE 1992-4209709 | 1992<br>0325      |
| PRIORITY APPLN. INFO.:                          |      |          | DE 1991-4135475 | A<br>1991<br>1028 |
|   |      |          | DE 1992-4209709 | A<br>1992<br>0325 |

AB The title polyurethanes, useful in slush molding, are prepared by the reaction of emulsions of components bearing free NCO groups (or NCO-reactive groups) with components bearing an average of 2 NCO-reactive groups in the presence of a sep. prepared component bearing blocked NCO groups in an inert organic liquid carrier. Adipic acid-hexanediol-neopentyl glycol polyester (OH number 56) 68.2 and HMDI 19.7 parts were heated to 80°, mixed with 3.6 parts reaction product of 800 parts HMDI isocyanurate trimer and 543.9 parts Et 4-hydroxybenzoate, 2 parts Bu<sub>2</sub>Sn dilaurate, 233 parts isoctane, and 7.8 parts 1,4-butanediol, stirred for 2 h at 90°, and cooled to give a free-flowing powder with particle size distribution 93.1% 100-315 µm and m.p. 160°. Heating a 1000-µm layer of this powder on glass at 200° for 20 min gave a film with tensile strength 27 MPa, elongation 751%, cut growth resistance 584 N/cm, and softening point 160°.

IT 151931-82-7  
 (powder, preparation of thermoplastic, from emulsions)

RN 151931-82-7 HCAPLUS

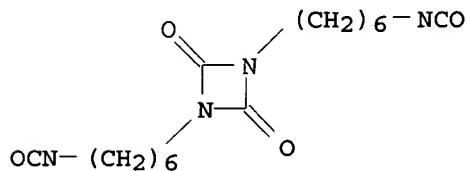
CN Hexanedioic acid, polymer with 1,3-bis(6-isocyanatohexyl)-1,3-

diazetidine-2,4-dione, 1,4-butanediol, 1,6-diisocyanatohexane, 2,2-dimethyl-1,3-propanediol and 1,6-hexanediol (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

CMF C16 H24 N4 O4



CM 2

CRN 822-06-0

CMF C8 H12 N2 O2

OCN- (CH<sub>2</sub>)<sub>6</sub> - NCO

CM 3

CRN 629-11-8

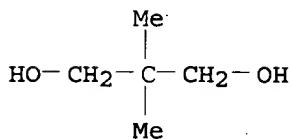
CMF C6 H14 O2

HO- (CH<sub>2</sub>)<sub>6</sub> - OH

CM 4

CRN 126-30-7

CMF C5 H12 O2



CM 5

CRN 124-04-9

CMF C6 H10 O4

HO2C-(CH2)4-CO2H

CM 6

CRN 110-63-4  
CMF C4 H10 O2

HO-(CH2)4-OH

IC ICM C08G018-08  
ICS C08G018-10; C08G018-80; C08G018-79; C08J003-24  
ICA C08L075-04  
CC 37-3 (Plastics Manufacture and Processing)  
IT 151931-81-6 151931-82-7 151931-83-8 151931-84-9  
(powder, preparation of thermoplastic, from emulsions)

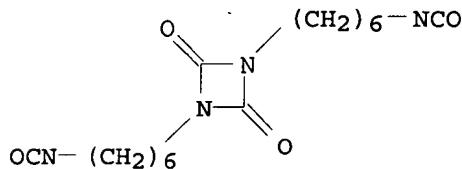
L50 ANSWER 21 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1993:604627 HCAPLUS  
DOCUMENT NUMBER: 119:204627  
TITLE: Polyisocyanate mixtures and their preparation and use as crosslinking agents in aqueous binder compositions  
INVENTOR(S): Reiff, Helmut  
PATENT ASSIGNEE(S): Bayer A.-G., Germany  
SOURCE: Ger. Offen., 9 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.                                   | KIND     | DATE                 | APPLICATION NO. | DATE              |
|--|----------|----------------------|-----------------|-------------------|
| DE 4129953                                   | A1       | 19930311             | DE 1991-4129953 | 1991<br>0910      |
| EP 531820                                    | A1       | 19930317             | EP 1992-114682  | 1992<br>0828      |
| EP 531820<br>R: DE, FR, GB, IT<br>CA 2077633 | B1<br>AA | 19970709<br>19930311 | CA 1992-2077633 | 1992<br>0904      |
| CA 2077633<br>US 5258452                     | C<br>A   | 20021119<br>19931102 | US 1992-940564  | 1992<br>0904      |
| PRIORITY APPLN. INFO.:                       |          |                      | DE 1991-4129953 | A<br>1991<br>0910 |

AB A polyisocyanate composition containing (cyclo)aliphatic isocyanate groups and having average NCO functionality

$\geq 2.1$  and a modifier containing  $\geq 1$  tertiary N and  $\geq 1$  isocyanate-reactive group are used to prepare a polyisocyanate mixture having an NCO functionality 2.3-4.3. The mixture is useful as a crosslinking composition, which forms stable aqueous emulsions. Reacting 50 g (2-hydroxyethyl)morpholine with 1 kg trimerized hexamethylene diisocyanate [mixture of tris(6-isocyanatoethyl) isocyanurate and higher homologs] having average NCO functionality 3.3 and adding 43.3 g Me<sub>2</sub>SO<sub>4</sub> gave a product (NCO content 17.9%; quaternary N content 32.7 mequiv./100 g), which was mixed (25 g) with 75 g water to give an emulsion showing storage stability  $>1$  day.

IT 23501-81-7DP, reaction products with amines (preparation of emulsifiable, as crosslinking agents)  
 RN 23501-81-7 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatoethyl)- (9CI) (CA INDEX NAME)



IC ICM C08G018-78  
 ICS C08G018-79; C08G018-48; C09D175-04; C09J175-04  
 ICI C09D175-04, C09D133-04; C09D167-00, C09D167-08  
 CC 37-6 (Plastics Manufacture and Processing)  
 ST isocyanate mixt prepn emulsion crosslinker;  
 hexamethylene diisocyanate trimer deriv crosslinker;  
 hydroxyethylmorpholine polyisocyanate mixt emulsion  
 crosslinker; polyisocyanate mixt prepn emulsion  
 crosslinker; quaternary ammonium polyisocyanate emulsion  
 crosslinker; amine polyisocyanate emulsion crosslinker;  
 binder emulsion crosslinker polyisocyanate; adhesive  
 emulsion crosslinker polyisocyanate;  
 polyurethane emulsion crosslinker polyisocyanate  
 IT Emulsifying agents  
 (amine-polyisocyanate reaction products, for  
 polyisocyanate mixts. as crosslinking agents)  
 IT Adhesives  
 Binding materials  
 Coating materials  
 (crosslinking agents for, emulsifiable polyisocyanate  
 mixts. as)  
 IT Emulsions  
 (of polyisocyanate mixts., as crosslinking agents)  
 IT Crosslinking agents  
 (polyisocyanates, emulsifiable, for adhesives and  
 coatings)  
 IT Urethane polymers, preparation  
 (preparation and crosslinking of, emulsifiable  
 polyisocyanates for)  
 IT Quaternary ammonium compounds, preparation  
 (preparation of isocyanate group-containing, emulsifiable, as  
 crosslinking agents)  
 IT 77-78-1DP, Dimethylsulfate, quaternization products with amine  
 derivs. of polyisocyanates 103-76-4DP,

N-(2-Hydroxyethyl)piperazine, reaction products with **polyisocyanates** 108-19-0DP, Biuret, **isocyanate** derivs., reaction products with amines 622-40-2DP, N-(2-Hydroxyethyl)morpholine, reaction products with **polyisocyanates** 822-06-0DP, Hexamethylene diisocyanate, biuret and isocyanurate derivs., reaction products with amines 3040-44-6DP, N-(2-Hydroxyethyl)piperidine, reaction products with **polyisocyanates** 3779-63-3DP, Tris(6-isocyanatohexyl) isocyanurate, reaction products with amines 4035-89-6DP, N,N',N''-Tris(6-isocyanatohexyl)biuret, reaction products with amines 4098-71-9DP, Isophorone diisocyanate, trimers, reaction products with amines 9003-11-6DP, Ethylene oxide-propylene oxide copolymer, reaction products with amino derivs. of **polyisocyanates** 9038-95-3DP, Ethylene oxide-propylene oxide copolymer monobutyl ether, reaction products with amino derivs. of **polyisocyanates** 14037-23-1DP, reaction products with **polyisocyanates** 23501-81-7DP, reaction products with amines 25322-68-3DP, Polyethylene glycol, reaction products with amino derivs. of **polyisocyanates** 76996-65-1DP, reaction products with amino derivs. of **polyisocyanates** (preparation of emulsifiable, as crosslinking agents)

L50 ANSWER 22 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:86069 HCPLUS

DOCUMENT NUMBER: 116:86069

TITLE: Syntheses and reactions of **urethanes** of cellobiose and cellulose-containing uretdione groups

AUTHOR(S): Meyer-Stork, L. Sebastian; Hoecker, Hartwig; Berndt, Heinz

CORPORATE SOURCE: RWTH Aachen, Aachen, 5100, Germany

SOURCE: Journal of Applied Polymer Science (1992), 44(6), 1043-9

CODEN: JAPNAB; ISSN: 0021-8995

DOCUMENT TYPE: Journal

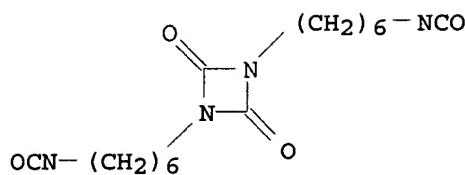
LANGUAGE: English

AB **Urethanes** of cellobiose and cellulose-containing uretdione groups are synthesized by the reaction of aliphatic and aromatic diisocyanate uretdiones with the saccharides. The syntheses are performed as a heterogeneous reaction in AcNMe<sub>2</sub> using dibutyltin dilaurate as catalyst, as well as a homogeneous reaction in AcNMe<sub>2</sub>-LiCl. Thus, semisynthetic prepolymers are formed that offer the reactivity of (blocked) **isocyanate** groups. To demonstrate their reactivity, ring opening of the uretdiones is performed by the addition of a secondary amine to yield the corresponding ureas.

IT 23501-81-7DP, Hexamethylene diisocyanate dimer, reaction products with cellobiose or cellulose (preparation and structural characterization of)

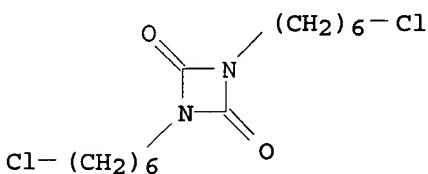
RN 23501-81-7 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



CC 43-3 (Cellulose, Lignin, Paper, and Other Wood Products)  
 Section cross-reference(s): 35  
 ST urethane cellobiose cellulose uretedione  
 IT 528-50-7DP, D-Cellobiose, reaction products with hexamethylene diisocyanate dimer or TDI dimer 9004-34-6DP, Cellulose, reaction products with hexamethylene diisocyanate dimer or TDI dimer 23501-81-7DP, Hexamethylene diisocyanate dimer, reaction products with cellobiose or cellulose 26747-90-0DP, TDI dimer, reaction products with cellobiose or cellulose (preparation and structural characterization of)

L50 ANSWER 23 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1988:529114 HCAPLUS  
 DOCUMENT NUMBER: 109:129114  
 TITLE: Synthesis and hydrolysis of (siloxyethyl)ureas  
 AUTHOR(S): Vostokov, I. A.; Vasyaeva, L. V.  
 CORPORATE SOURCE: Gos. Nauchno-Issled. Inst. Azotn. Prom., Dzerzhinsk, USSR  
 SOURCE: Zhurnal Obshchey Khimii (1987), 57(10), 2329-33  
 CODEN: ZOKHA4; ISSN: 0044-460X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 OTHER SOURCE(S): CASREACT 109:129114  
 AB 3,4-C<sub>12</sub>C<sub>6</sub>H<sub>3</sub>NHCONRCH<sub>2</sub>CH<sub>2</sub>OSiMe<sub>3</sub> (R = H, CH<sub>2</sub>CH<sub>2</sub>OSiMe<sub>3</sub>, SiMe<sub>3</sub>) were prepared in 95-100% yields by treating 3,4-C<sub>12</sub>C<sub>6</sub>H<sub>3</sub>NCO with R<sub>1</sub>NHCH<sub>2</sub>CH<sub>2</sub>OSiMe<sub>3</sub>. Hydrolysis of R<sub>1</sub>NHCONRCH<sub>2</sub>CH<sub>2</sub>OSiMe<sub>3</sub> [R<sub>1</sub> = C<sub>1</sub>(CH<sub>2</sub>)<sub>6</sub>, 3-C<sub>1</sub>C<sub>6</sub>H<sub>4</sub>, 3,4-C<sub>12</sub>C<sub>6</sub>H<sub>3</sub>; R = H, CH<sub>2</sub>CH<sub>2</sub>OSiMe<sub>3</sub>] gave 61-100% R<sub>1</sub>NHCONRCH<sub>2</sub>CH<sub>2</sub>OH.  
 IT 23336-46-1P (preparation of)  
 RN 23336-46-1 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-chlorohexyl)- (9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)  
 ST addn isocyanate siloxyethylamine; siloxyethylurea; urea siloxyethyl phenyl; hydrolysis siloxyethylurea; hydroxyethylurea  
 IT Addition reaction (of Ph isocyanates with siloxyethylamines, siloxyethylureas by)

IT 1025-36-1P 1785-02-0P 3420-84-6P 4459-90-9P 15145-34-3P  
 16122-64-8P 23336-46-1P 23544-79-8P 69796-24-3P  
 87919-35-5P 91933-84-5P 116422-02-7P 116422-03-8P  
 116422-04-9P  
 (preparation of)  
 IT 20836-42-4  
 (reaction of, with Ph isocyanate)  
 IT 17165-52-5  
 (reaction of, with Ph isocyanate derivs.)  
 IT 111-42-2, Diethanolamine, reactions 5804-92-2 20836-40-2  
 (reaction of, with dichlorophenyl isocyanate)  
 IT 102-36-3 103-71-9, Phenyl isocyanate, reactions  
 2909-38-8 13654-91-6, 6-Chlorohexyl isocyanate  
 (reaction of, with siloxyethylamines)

L50 ANSWER 24 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:511355 HCAPLUS

DOCUMENT NUMBER: 109:111355

TITLE: Analysis of chemical structures of isocyanurate-oxazolidone resins by infrared absorption spectroscopy

AUTHOR(S): Yokoyama, Takashi; Koyama, Toru; Kinjo, Noriyuki; Narahara, Toshikazu

CORPORATE SOURCE: Hitachi Res. Lab., Hitachi Ltd., Hitachi, 319-12, Japan

SOURCE: Kobunshi Ronbunshu (1988), 45(6), 491-8  
 CODEN: KBRBA3; ISSN: 0386-2186

DOCUMENT TYPE: Journal

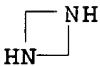
LANGUAGE: Japanese

AB Isocyanurate-oxazolidone resins were prepared from 2,4-TDI and 2,2-bis[p-(2,3-epoxypropoxy)phenyl]propane (I) using N-methylmorpholine as a catalyst. Model polymers containing isocyanurate, oxazolidone, and uretidindione rings were prepared from TDI, MDI, tri-Ph isocyanate, and I in order to form calibration curves for IR spectra. Composition of hetero rings in the cured product varied with curing temperature, time, and compound ratio. Isocyanate groups changed mainly to isocyanurate rings with .apprx.20 mol% of the groups becoming oxazolidone rings. Product contents of uretidindione rings were <6 mol%. Reaction routes were analyzed from conversion ratios. Variations in the bending strength of the resins made from modified MDI and I are discussed in relation to hetero ring content.

IT 5663-08-1DP, 1,3-Diazetidine, derivs., polymers  
 (preparation of, from diisocyanates and bis(epoxypropylphenyl)propane, hetero ring formation in, effect of curing conditions on)

RN 5663-08-1 HCAPLUS

CN 1,3-Diazetidine (9CI) (CA INDEX NAME)



CC 37-4 (Plastics Manufacture and Processing)

IT Ring closure and formation  
 (in polymerization of diisocyanates and bis(epoxypropylphenyl)propane)

IT Polymerization

(of diisocyanates with bis[(epoxypropyl)phenyl]propane, mechanism of oxazolidone and isocyanurate and uretidindione ring formation in)

IT Chains, chemical  
(structure of, of diisocyanate-  
bis(epoxypropylphenyl)propane copolymers, effect of curing  
conditions on)

IT 504-76-7DP, Oxazolidine, derivs., polymers 5663-08-1DP,  
1,3-Diazetidine, derivs., polymers  
(preparation of, from diisocyanates and  
bis(epoxypropylphenyl)propane, hetero ring formation in, effect  
of curing conditions on)

L50 ANSWER 25 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:406994 HCAPLUS

DOCUMENT NUMBER: 109:6994

TITLE: Formation of a uretonimine in the production  
of heat-treated 4,4'-diphenylmethane  
diisocyanate

AUTHOR(S): Ivanov, M. G.; Golov, V. G.; Rogulev, V. A.;  
Mushkin, Yu. I.; Vodop'yanov, V. G.; Gerega,  
V. F.

CORPORATE SOURCE: USSR

SOURCE: Khimicheskaya Promyshlennost (Moscow, Russian  
Federation) (1988), (4), 208-10

CODEN: KPRMAW; ISSN: 0023-110X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 109:6994

AB In the thermal decarboxylation of MDI to give carbodiimide monomers containing NCO groups, a substituted uretonimine (1,3-diazacyclobutane derivative) was formed from reaction of the carbodiimide moiety with NCO groups of the MDI or the carbodiimide. The reaction was reversible at 120-180°. At 70° and lower, the reaction equilibrium shifted almost completely to the side of uretonimine formation. At 120° the equilibrium reaction mixture contained significant amts. of carbodiimide, resulting in a decrease in the content of trifunctional uretonimine and in a decrease of product functionality to 2. Kinetic data are given for the equilibrium reaction, and permit calcn. of the time necessary for achieving stable physicochem. properties of the product. Thus, 90-95% conversion of carbodiimide to uretonimine was achieved after 10-15 days at 20° or after 5-7 h at 70°.

IT 5663-08-1DP, 1,3-Diazacyclobutane, derivs.  
(formation of, in thermal decarboxylation of MDI to carbodiimide, kinetics and equilibrium of)

RN 5663-08-1 HCAPLUS

CN 1,3-Diazetidine (9CI) (CA INDEX NAME)

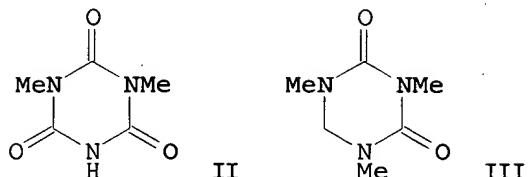


CC 35-2 (Chemistry of Synthetic High Polymers)

IT 5663-08-1DP, 1,3-Diazacyclobutane, derivs.

(formation of, in thermal decarboxylation of MDI to carbodiimide, kinetics and equilibrium of)

L50 ANSWER 26 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1986:552526 HCPLUS  
 DOCUMENT NUMBER: 105:152526  
 TITLE: Studies of methyl isocyanate  
 chemistry in the Bhopal incident  
 AUTHOR(S): D'Silva, Themistocles D. J.; Lopes, Anibal;  
 Jones, Russell L.; Singhawangcha, Sureerat;  
 Chan, John K.  
 CORPORATE SOURCE: Res. Dev. Dep., Union Carbide Agric. Prod.  
 Co., Inc., Research Triangle Park, NC, 27709,  
 USA  
 SOURCE: Journal of Organic Chemistry (1986), 51(20),  
 3781-8  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 105:152526  
 GI

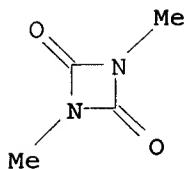


AB Following the MeNCO leak from Tank 610 at the Bhopal plant, the residual material from the tank was analyzed for its contents. Approx. 70% of the residue was comprised of 3 cyclic materials: MeNCO cyclotrimer, di-Me isocyanurate (I), and dihydrotr trimethyltriazinedione (II). Minor quantities of methyl-substituted ureas, biurets, and amine hydrochlorides were also found. The composition of the residue was replicated very closely by the products obtained when a mixture of MeNCO (84.4%), CHCl<sub>3</sub> (12.0%), and water (3.6%) was heated at 225° under pressure in a stainless steel reactor. Exptl. results are consistent with the view that under these conditions MeNCO reacts initially with water to form 1,3-dimethylurea (III) and 1,3,5-trimethylbiuret (IV). At 100-225° these products decompose to reactive intermediates which further react exothermically to form the aforementioned cyclic materials, trimethylurea, and mono-, di-, and trimethylamine hydrochlorides. The decomposition of III and IV is facilitated by the presence of CHCl<sub>3</sub> and metals. Other expts. involving <sup>13</sup>C-enriched CHCl<sub>3</sub> support the proposed mechanisms for formation of I and II.

IT 36909-44-1P  
 (preparation and detection of, Me isocyanate chemical and  
 Bhopal incident in relation to)

RN 36909-44-1 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-dimethyl- (9CI) (CA INDEX NAME)



CC 23-21 (Aliphatic Compounds)

ST methyl **isocyanate** chem Bhopal; cyclotrimerization methyl **isocyanate**; triazinetrione methylated; isocyanurate dimethyl; triazinedione dihydrotrimethyl

IT Trimerization  
(cyclo-, of Me **isocyanate**, Bhopal incident in relation to)

IT 75-44-5  
(Me **isocyanate** reactions in presence of, Bhopal incident in relation to)

IT 96-31-1  
(detection and reactions of, Me **isocyanate** chemical and Bhopal incident in relation to)

IT 506-59-2 593-51-1 593-81-7 632-22-4 7439-89-6, analysis  
7440-02-0, analysis 7440-47-3, analysis  
(detection of, Me **isocyanate** chemical and Bhopal incident in relation to)

IT 67-66-3, uses and miscellaneous  
(effect of, on Me **isocyanate** chemical)

IT 6452-47-7  
(preparation and Me **isocyanate** reactions in presence of, Bhopal incident in relation to)

IT 13188-08-4P  
(preparation and cyclocondensation of, Me **isocyanate** dimer from)

IT 827-16-7P 6726-48-3P 36909-44-1P 41221-01-6P.  
54070-65-4P  
(preparation and detection of, Me **isocyanate** chemical and Bhopal incident in relation to)

IT 632-14-4P 816-00-2P  
(preparation, detection, and reaction of, Me **isocyanate** chemical and Bhopal incident in relation to)

IT 31717-44-9  
(reaction of, with Me **isocyanate**, Bhopal incident in relation to)

IT 590-28-3  
(reaction of, with Me **isocyanate**, dimethyltriazinetrione from)

L50 ANSWER 27 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1983:488088 HCAPLUS

DOCUMENT NUMBER: 99:88088

TITLE: Synthesis of carbamoyl **isocyanates**  
by the exchange reaction of carbamoyl  
chlorides with trimethylisocyanatosilane\*  
\*\*

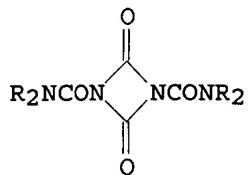
AUTHOR(S): Kozyukov, V. P.; Mironov, V. F.

CORPORATE SOURCE: Gos. Nauchno-Issled. Inst. Khim. Tekhnol.  
Elementoorg. Soedin., Moscow, USSR

SOURCE: Zhurnal Obshchey Khimii (1983), 53(6), 1434-5

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 OTHER SOURCE(S): CASREACT 99:88088  
 GI

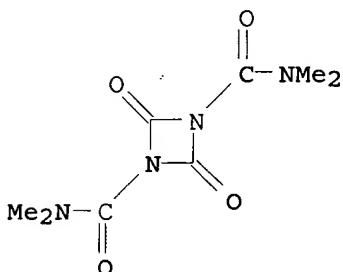


AB R<sub>2</sub>NC(O)NCO (I, R = Me, Et) are prepared in 70-90% yields by treatment of R<sub>2</sub>NCOCl with Me<sub>3</sub>SiNCO in the presence of SnCl<sub>4</sub> 3-5 h. I readily dimerize to give II which can be decomposed to the monomer at 200-300° and 2-3 mm pressure.

IT \*\*\*68661-66-5P 86790-60-5P  
 (preparation and conversion to monomer)

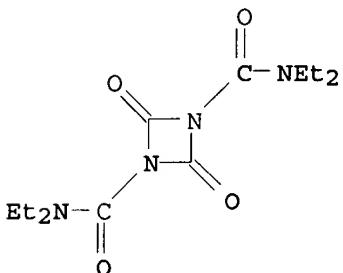
RN 68661-66-5 HCPLUS

CN 1,3-Diazetidine-1,3-dicarboxamide, N,N,N',N'-tetramethyl-2,4-dioxo-  
 (9CI) (CA INDEX NAME)



RN 86790-60-5 HCPLUS

CN 1,3-Diazetidine-1,3-dicarboxamide, N,N,N',N'-tetraethyl-2,4-dioxo-  
 (9CI) (CA INDEX NAME)



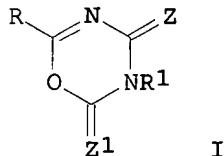
CC 28-4 (Heterocyclic Compounds (More Than One Hetero Atom))

ST diazetidinedione; *isocyanate* dimethylcarbamoyl  
 cyclodimerization

IT Condensation reaction  
 (of carbamoyl chlorides with trimethylsilyl *isocyanate*)

)  
 IT Dimerization  
 (cyclo-, of dialkylcarbamoyl **isocyanates**)  
 IT 68661-66-5P 86790-60-5P  
 (preparation and conversion to monomer)  
 IT 79-44-7 88-10-8  
 (reaction of, with trimethylsilyl **isocyanate**)

L50 ANSWER 28 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1981:462141 HCAPLUS  
 DOCUMENT NUMBER: 95:62141  
 TITLE: Cycloaddition reactions between acyl (or thioacyl) **isocyanates** (or **isothiocyanates**) and **isocyanates** (or **isothiocyanates**)  
 AUTHOR(S): Raton, Serge; Moyne, Jose; Longeray, Remi  
 CORPORATE SOURCE: Cent. Rech. Decines, Rhone-Poulenc Rech. Dev., Decines-Charpieu, 69150, Fr.  
 SOURCE: Bulletin de la Societe Chimique de France (1981), (1-2, Pt. 2), 28-32  
 DOCUMENT TYPE: CODEN: BSCFAS; ISSN: 0037-8968  
 LANGUAGE: Journal  
 French  
 OTHER SOURCE(S): CASREACT 95:62141  
 GI



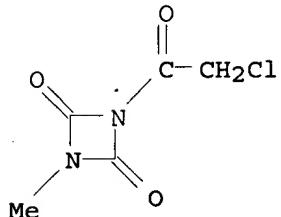
AB The reaction of RCONCZ [R = Ph, O2NC6H4, 2,4-Me(Cl)C6H3OCH2, 4,3,5-Cl(O2N)2C6H2, ClCH2, PhOCH2, Me2N; Z = O, S] with R1NCZ1 (R1 = Me, Et, Ph, 4-FC6H4; Z1 = O, S) gave oxadiazines I. Thus, PhCONCO was added MeNCO in ether at 20°, and the mixture was stirred 120 h to give I (Z = Z1 = O, R = Ph, R1 = Me).

IT 78488-11-6P

(preparation of)

RN 78488-11-6 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1-(chloroacetyl)-3-methyl- (9CI) (CA INDEX NAME)



CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 23, 25

ST oxadiazinedione; cycloaddn benzoyl **isocyanate**; methyl **isocyanate** cycloaddn  
 IT Cycloaddition reaction  
     (of acyl **isocyanates** and carbamoyl isothiocyanate derivative with organic **isocyanates** and isothiocyanates, oxadiazines and thiadiazines from)  
 IT 4461-30-7 4461-31-8 4461-37-4 5843-49-2 41835-30-7  
     61831-98-9  
     (cycloaddn. reaction of, with Me **isocyanate**)  
 IT 103-71-9, reactions 109-90-0  
     (cycloaddn. reaction of, with benzoyl **isocyanate** and carbamoyl isothiocyanate derivative)  
 IT 624-83-9  
     (cycloaddn. reaction of, with benzoyl **isocyanates** and carbamoyl isothiocyanate derivative)  
 IT 4461-33-0  
     (cycloaddn. reaction of, with organic **isocyanates**)  
 IT 16011-79-3  
     (cycloaddn. reaction of, with organic **isocyanates** and isothiocyanates)  
 IT 61831-87-6P 61831-88-7P 61831-89-8P 61831-90-1P  
     61831-91-2P 61831-92-3P 61831-94-5P 61831-95-6P  
     61831-96-7P 61831-97-8P 78488-10-5P **78488-11-6P**  
     78488-12-7P 78488-13-8P 78488-14-9P 78488-15-0P  
     (preparation of)

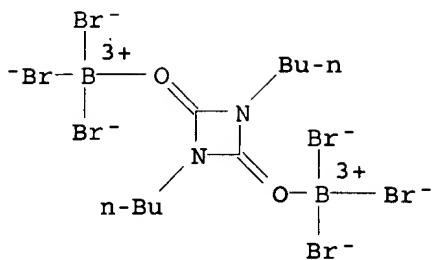
L50 ANSWER 29 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1980:75625 HCPLUS  
 DOCUMENT NUMBER: 92:75625  
 TITLE: Coordination properties of **isocyanates**  
 AUTHOR(S): Varentsova, N. V.; Gol'dshtein, I. P.;  
               Shufrina, R. R.; Shcherbakova, E. S.;  
               Tarakanov, O. G.; Gur'yanova, E. N.  
 CORPORATE SOURCE: Nauchno-Issled. Fiz.-Khim. Inst. im. Karpova,  
                   Moscow, USSR  
 SOURCE: Zhurnal Obshchey Khimii (1979), 49(9), 2082-90  
 CODEN: ZOKHA4; ISSN: 0044-460X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian

AB Calorimetric, cryoscopic and spectral data indicated that BuNCO and PhNCO formed complexes with electron acceptors, e.g., SnCl<sub>4</sub>, CF<sub>3</sub>CO<sub>2</sub>H, BBr<sub>3</sub> and AlBr<sub>3</sub>. The last 2 compds. also formed complexes with cyclic dimers and trimers of the **isocyanates**. The heats of formation of 2:1 complexes of AlBr<sub>3</sub> with BuNCO and PhNCO were -28.3 and -17.2 kcal/mol, resp.; the values for the corresponding BBr<sub>3</sub> complexes were -25.5 and -14.3 kcal/mol. The **isocyanates** did not form complexes with tertiary amine donors.

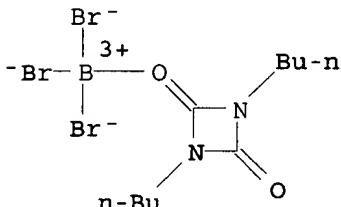
IT 72606-17-8P 72606-20-3P  
     (preparation of)

RN 72606-17-8 HCPLUS

CN Boron, hexabromo[ $\mu$ -(1,3-dibutyl-1,3-diazetidine-2,4-dione-O:O')]di- (9CI) (CA INDEX NAME)



RN 72606-20-3 HCPLUS

CN Boron, tribromo(1,3-dibutyl-1,3-diazetidine-2,4-dione-O)-, (T-4)-  
(9CI) (CA INDEX NAME)

CC 22-8 (Physical Organic Chemistry)

ST isocyanate complex electron acceptor; tin chloride complex isocyanate; aluminum bromide complex isocyanate; boron bromide complex isocyanate; fluoroacetic acid complex isocyanate

IT Ultraviolet and visible spectra  
(of isocyanate complexes with aluminum bromide)IT Infrared spectra  
(of isocyanate complexes with boron bromide)IT Molecular association  
(of isocyanates with electron acceptors)IT 110-86-1, reactions 121-44-8, reactions 280-57-9  
(attempted complexation of, with isocyanates)IT 7727-15-3 10294-33-4  
(complexation of, with isocyanates)IT 72576-88-6P 72576-89-7P 72576-90-0P 72606-14-5P  
72606-15-6P 72606-16-7P 72606-17-8P 72606-18-9P  
72606-19-0P 72606-20-3P 72606-21-4P 72606-22-5P  
72606-23-6P 72606-24-7P 72627-57-7P  
(preparation of)

L50 ANSWER 30 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1979:22234 HCPLUS

DOCUMENT NUMBER: 90:22234

TITLE: Synthesis and properties of  
(N,N-dimethyl)dichloromethaniminium  
chlorosulfateAUTHOR(S): Kukhar, V. P.; Pasternak, V. I.; Shevchenko,  
M. V.

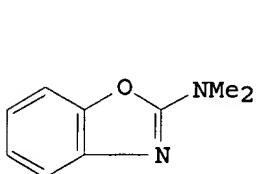
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1978), 14(9),  
1841-6

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE :  
LANGUAGE :  
OTHER SOURCE (S) :  
GI

Journal  
Russian  
CASREACT 90:22234



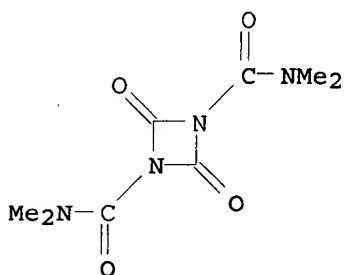
AB C12C:NMe<sub>2</sub>+ X- [I; X = Cl (II)] reacted with Me<sub>2</sub>SO<sub>4</sub> to give I [X = ClSO<sub>3</sub> (III)] via the intermediate I [X = MeOSO<sub>3</sub> (IV)]. III was also prepared directly from II in 81% yield by treatment with ClSO<sub>3</sub>H, and along with I (X = ClSO<sub>3</sub>SO<sub>3</sub>) by treatment with SO<sub>3</sub>. Analogously, Z:NMe<sub>2</sub>+ X- (V; Z = CH<sub>2</sub>, ClCH; X = Cl) reacted with SO<sub>3</sub> to give 85-96% V (Z = same; X = ClSO<sub>3</sub>, ClSO<sub>3</sub>SO<sub>3</sub>). Pyrolysis of III gave 80% Me<sub>2</sub>NCOC<sub>1</sub>, SO<sub>2</sub> and Cl<sub>2</sub>. III and IV cyclized with o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>OH to give benzoxazole VI. III reacted with p-ClC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>NC<sub>1</sub> to give 41% p-ClC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>N:CClNMe<sub>2</sub>, and with Cl<sub>2</sub>NCO<sub>2</sub>Et to give 83% Me<sub>2</sub>NCONCO, which underwent partial cyclodimerization to VI on distillation and reacted with PhNH<sub>2</sub> to give Me<sub>2</sub>NCONHC<sub>6</sub>H<sub>4</sub>NHPh.

IT 68661-66-5P

(preparation of)

RN 68661-66-5 HCAPLUS

CN 1,3-Diazetidine-1,3-dicarboxamide, N,N,N',N'-tetramethyl-2,4-dioxo-  
(9CI) (CA INDEX NAME)



## CC 23-4 (Aliphatic Compounds)

Section cross-reference(s) : 28

IT 62-53-3, reactions

(addition reaction of, with dimethylcarbamoyl **isocyanate**)

IT 2617-87-0P 13858-89-4P 34520-13-3P 68661-60-9P 68661-62-1P

68661-66-5P 68661-67-6P

(preparation of)

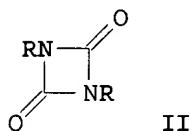
L50 ANSWER 31 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:615264 HCAPLUS

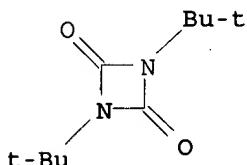
ACCESSION NUMBER: 1978.0152  
DOCUMENT NUMBER: 89:215264

**TITLE:** Synthesis of 1,3-dialkyldiazetidinediones from

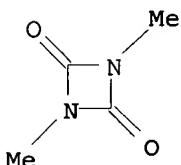
AUTHOR(S): N,N'-dialkylaminocarbonylcarbamic chlorides  
 (2,4-dialkylallophanoyl chlorides)  
 White, Dabney K.; Greene, Frederick D.  
 Dep. Chem., Massachusetts Inst. Technol.,  
 Cambridge, MA, USA  
 SOURCE: Journal of Organic Chemistry (1978), 43(23),  
 4530-2  
 DOCUMENT TYPE: CODEN: JOCEAH; ISSN: 0022-3263  
 LANGUAGE: Journal  
 English  
 OTHER SOURCE(S): CASREACT 89:215264  
 GI



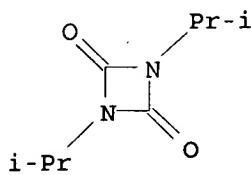
AB Hydrolyzing the title carbamoyl chlorides, RN:CClNRCOCl (R = CHMe<sub>2</sub>, cyclohexyl, CMe<sub>3</sub>) in acetone-water gave 60-80% RNHCONRCOCl (I). Treating I with 1,4-diazabicyclo[2.2.2]octane in ether gave 55-84% 1,3-dialkyl-2,4-diazetidinediones II (R = CHMe<sub>2</sub>, cyclohexyl, CMe<sub>3</sub>, Me). Use of NaH or KOCMe<sub>3</sub> to promote ring closure of I gave mixts. of products.  
 IT 30885-14-4P 36909-44-1P 67463-80-3P  
 (preparation of)  
 RN 30885-14-4 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



RN 36909-44-1 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 67463-80-3 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

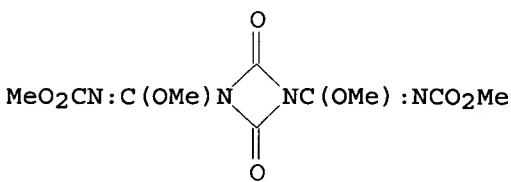


CC 28-4 (Heterocyclic Compounds (More Than One Hetero Atom))  
 IT 15234-14-7P 30885-14-4P 36909-44-1P  
 51170-55-9P 67463-80-3P 67463-81-4P  
 (preparation of)  
 IT 75-65-0, reactions  
 (reaction of, with iso-Pr isocyanate)

L50 ANSWER 32 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1978:6583 HCAPLUS  
 DOCUMENT NUMBER: 88:6583  
 TITLE: Alkoxy carbonylisourea isocyanates  
 INVENTOR(S): Fuchs, Julius Jakob  
 PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA  
 SOURCE: U.S., 5 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE               |
|------------------------|------|----------|-----------------|--------------------|
| US 4045473             | A    | 19770830 | US 1975-603651  | 1975<br>0811       |
| US 4075201             | A    | 19780221 | US 1977-776258  | 1977<br>0310       |
| PRIORITY APPLN. INFO.: |      |          | US 1975-603651  | A3<br>1975<br>0811 |

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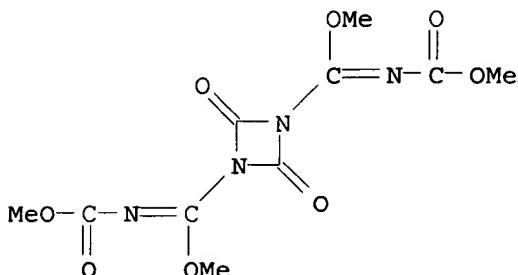


AB MeO<sub>2</sub>CN:C(OMe)NH<sub>2</sub>, prepared from MeOC(NH<sub>2</sub>):NH and MeO<sub>2</sub>CCl, was treated with Cl<sub>2</sub>CO to give the diazepidine biscarbamate I via MeO<sub>2</sub>CN:C(OMe)NCO. I was treated with cyclohexylamine to give RNHCONHC(OMe):NCO<sub>2</sub>Me (II, R = cyclohexyl). II (R = p-ClC<sub>6</sub>H<sub>4</sub>) was similarly prepared II were herbicidal (no data).  
 IT 64836-49-3P

(preparation and reaction with amines)

RN 64836-49-3 HCPLUS

CN 1,3-Diazetidine-1,3-dicarboximidic acid, N,N'-bis(methoxycarbonyl)-2,4-dioxo-, dimethyl ester (9CI) (CA INDEX NAME)



IC C07C127-26

INCL 260482000C

CC 25-28 (Noncondensed Aromatic Compounds)

Section cross-reference(s): 5

ST allophanimide prepn herbicide; diazetidine biscarbamate; isocyanate alkoxycarbonylisourea

IT 64836-49-3P

(preparation and reaction with amines)

L50 ANSWER 33 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:423111 HCPLUS

DOCUMENT NUMBER: 87:23111

TITLE: 1,3-Dialkyldiazetidin-2,4-diones. Structure and molecular spectra

AUTHOR(S): Kuhn, Norbert; Schwarz, Wolfgang; Schmidt, Armin

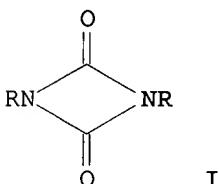
CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Stuttgart, Stuttgart, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1977), 110(3), 1130-9  
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



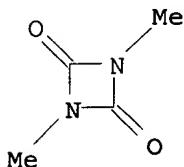
AB Diazetidinediones I (R = Me, Et) were prepared by cyclizing dimerization of the corresponding RNCO (R = Me, Et) with SbCl5. The vibrational spectra of I (R = Me, Et) were discussed. The crystal and mol. structure of I (R = Me) were determined, as well as 1H NMR data for I (R = Me, Et).

IT 36909-44-1P

(preparation and crystal and mol. structure and spectra of)

RN 36909-44-1 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-dimethyl- (9CI) (CA INDEX NAME)

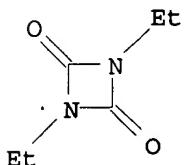


IT 23336-34-7P

(preparation and spectra of)

RN 23336-34-7 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-diethyl- (9CI) (CA INDEX NAME)



CC 28-4 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 22, 75

ST alkyl isocyanate cyclodimerization; diazetidinedione  
crystal mol structure; vibrational spectra diazetidinedione; NMR  
diazetidinedione

IT 7647-18-9

(cyclodimerization of alkyl isocyanates in presence  
of)

IT 36909-44-1P

(preparation and crystal and mol. structure and spectra of)

IT 23336-34-7P

(preparation and spectra of)

L50 ANSWER 34 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:190109 HCPLUS

DOCUMENT NUMBER: 86:190109

TITLE: Trialkyl- and triaryl(isocyanatomethyl  
chlorophosphoranesAUTHOR(S): Kozhushko, B. N.; Gumenyuk, A. V.; Paliichuk,  
Yu. A.; Shokol, V. A.

CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR

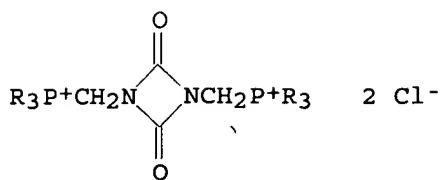
SOURCE: Zhurnal Obshchey Khimii (1977), 47(2), 333-9

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI

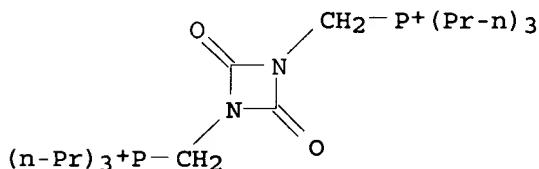


AB R3P+CH2NCO Cl- (I; R = Ph, p-MeOC<sub>6</sub>H<sub>4</sub>, p-MeC<sub>6</sub>H<sub>4</sub>) and II (R = Pr, octyl, decyl) were prepared in 84-96% yields by treating R3P with ClCH<sub>2</sub>NCO in ether at 0-10°. I dimerized in the presence of Pr<sub>3</sub>P in CHCl<sub>3</sub> to give the corresponding aryl dimers II. Treating I or II with R1OH gave 12 R3P+CH<sub>2</sub>NHCO<sub>2</sub>R1 Cl- (R1 = Me, Et, Pr, Me<sub>2</sub>CH, Bu, Ph,  $\alpha$ -naphthyl) in 50-92% yield.

IT 62779-07-1P 62779-08-2P 62779-09-3P  
(preparation and reaction with alcs.)

RN 62779-07-1 HCAPLUS

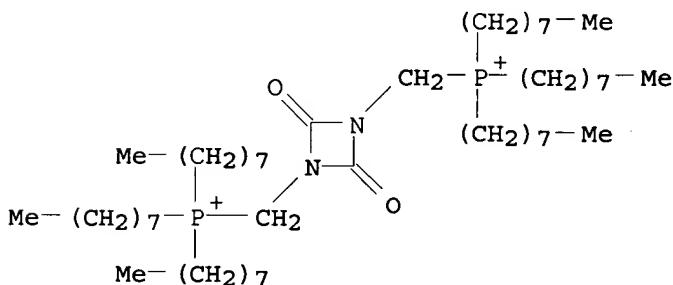
CN Phosphonium, [(2,4-dioxo-1,3-diazetidine-1,3-diyl)bis(methylene)]bis[tripropyl-, dichloride (9CI) (CA INDEX NAME)



●<sub>2</sub> Cl<sup>-</sup>

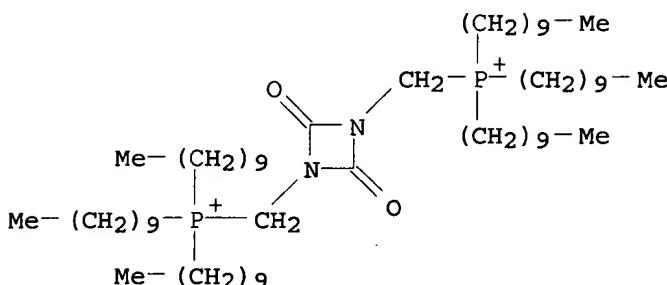
RN 62779-08-2 HCAPLUS

CN Phosphonium, [(2,4-dioxo-1,3-diazetidine-1,3-diyl)bis(methylene)]bis[trioctyl-, dichloride (9CI) (CA INDEX NAME)



●<sub>2</sub> Cl<sup>-</sup>

RN 62779-09-3 HCAPLUS  
 CN Phosphonium, [(2,4-dioxo-1,3-diazetidine-1,3-diyl)bis(methylene)]bis[tris(decyl)-, dichloride (9CI) (CA INDEX NAME)



●2 Cl<sup>-</sup>

CC 29-7 (Organometallic and Organometalloidal Compounds)  
 ST phosphonium isocyanatomethyl alkyl aryl; phosphorane  
 isocyanatomethyl alkyl aryl; isocyanate  
 phosphorane  
 IT Alcohols, reactions  
 (reaction of, with isocyanatomethylphosphonium  
 chlorides)  
 IT 21955-22-6P 62779-07-1P 62779-08-2P  
 62779-09-3P 62779-10-6P 62779-11-7P 62779-12-8P  
 62779-13-9P 62779-14-0P  
 (preparation and reaction with alcs.)  
 IT 603-35-0, reactions 855-38-9 1038-95-5 2234-97-1 4731-53-7  
 17621-07-7  
 (reaction of, with chloromethyl isocyanate)  
 IT 64-17-5, reactions 67-56-1, reactions 67-63-0, reactions  
 71-23-8, reactions 71-36-3, reactions 108-95-2, reactions  
 1321-67-1  
 (reaction of, with isocyanatomethylphosphonium  
 chlorides)

L50 ANSWER 35 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1976:509180 HCAPLUS  
 DOCUMENT NUMBER: 85:109180  
 TITLE: Thermostable polymers obtained by  
 heating an aromatic imine with a  
 polyisocyanate  
 INVENTOR(S): Balme, Maurice; Gruffaz, Max; Rollet, Bernard  
 PATENT ASSIGNEE(S): Societe des usines chimiques de Rhone-Poulenc,  
 Fr.  
 SOURCE: Fr. Demande, 20 pp.  
 CODEN: FRXXBL  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|------|-----------------|------|
|------------|------|------|-----------------|------|

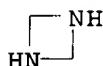
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 FR 2279780 A1 19760220 FR 1974-25386  
 1974  
 0722  
 FR 2279780 B1 19770325 FR 1974-25386 A  
 PRIORITY APPLN. INFO.: 1974  
 0722

AB Polymers resistant to heating at  $\leq 180^\circ$  were prepared by treating 4,4'-diisocyanatodiphenylmethane (I) with a benzylideneaminobenzene and optionally a bismaleimide. A mixture of 75.8 g 4,4'-bis(benzylideneamino)methane and 50 g I was heated 135 min at  $260^\circ$  and 5.8 g CO<sub>2</sub> was evolved. A polyimine diisocyanate was obtained which softened at 176-80° and 50 g of this polymer was treated with 150 g 4,4'-bis(maleimido)diphenylmethane and heated 30 min at 165-70° to give a polymer softening at 148-50° which was molded in 1 hr at  $250^\circ$  and 200 bars to give a product with initial flexural strength 5.1 kg/mm<sup>2</sup> and flexural modulus 232 kg/mm<sup>2</sup> which changed to 6.8, 6.5, and 6.7 kg/mm<sup>2</sup> and 266, 257, and 226 kg/mm<sup>2</sup> for strength and modulus resp., after 1160, 2230, and 3250 hr at  $250^\circ$ .

IT 5663-08-1DP, 1,3-Diazetidine, derivs., polymers  
 (heat-resistant)

RN 5663-08-1 HCPLUS

CN 1,3-Diazetidine (9CI) (CA INDEX NAME)



IC C08G033-02  
 CC 35-3 (Synthetic High Polymers)  
 ST benzylideneamino arom isocyanate polymer; polyimine polyisocyanate prep; heat resistant polyimine isocyanate  
 IT Heat-resistant materials  
 (aromatic imine-aromatic diisocyanate polymers)  
 IT 5663-08-1DP, 1,3-Diazetidine, derivs., polymers  
 55719-52-3 55719-53-4 55753-37-2  
 (heat-resistant)

L50 ANSWER 36 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1976:91789 HCPLUS  
 DOCUMENT NUMBER: 84:91789  
 TITLE: Polyaddition products containing uretdione groups  
 INVENTOR(S): Mueller, Hanns P.; Wagner, Kuno; Mueller, Richard  
 PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 36 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.               | KIND     | DATE                 | APPLICATION NO. | DATE              |
|--------------------------|----------|----------------------|-----------------|-------------------|
| DE 2420475               | A1       | 19751106             | DE 1974-2420475 | 1974<br>0427      |
| DE 2420475<br>AU 7579786 | C2<br>A1 | 19871203<br>19761007 | AU 1975-79786   | 1975<br>0403      |
| CA 1084196               | A1       | 19800819             | CA 1975-223960  | 1975<br>0407      |
| US 4044171               | A        | 19770823             | US 1975-569112  | 1975<br>0417      |
| DK 7501793               | A        | 19751028             | DK 1975-1793    | 1975<br>0424      |
| SE 7504773               | A        | 19751028             | SE 1975-4773    | 1975<br>0424      |
| NL 7504862               | A        | 19751029             | NL 1975-4862    | 1975<br>0424      |
| GB 1492102               | A        | 19771116             | GB 1975-17005   | 1975<br>0424      |
| BE 828385                | A1       | 19751027             | BE 1975-155767  | 1975<br>0425      |
| FR 2268840               | A1       | 19751121             | FR 1975-13112   | 1975<br>0425      |
| FR 2268840<br>BR 7502548 | B1<br>A  | 19790330<br>19760303 | BR 1975-3232    | 1975<br>0425      |
| ES 436992                | A1       | 19770116             | ES 1975-436992  | 1975<br>0425      |
| AT 7503187               | A        | 19770515             | AT 1975-3187    | 1975<br>0425      |
| AT 341221<br>CH 616169   | B<br>A   | 19780125<br>19800314 | CH 1975-5330    | 1975<br>0425      |
| JP 50149793              | A2       | 19751201             | JP 1975-50261   | 1975<br>0426      |
| JP 57046447              | B4       | 19821004             |                 |                   |
| PRIORITY APPLN. INFO.:   |          |                      | DE 1974-2420475 | A<br>1974<br>0427 |

AB Dimerization of diisocyanates in the presence of Bu<sub>3</sub>P or dibutyltin dilaurate (I) and polymerization with diols gave uretdione group-containing polyurethanes useful as hardeners for powdered

polyester-based coating materials. Thus, a mixture of 2,4-tolylene diisocyanate 313.2, MeOCH<sub>2</sub>CH<sub>2</sub>OAc 975, PhMe 325, and Bu<sub>3</sub>P 7.2 parts was stirred for 3.5 hr at 10-15°, treated with 10% S solution in PhMe 22.8 hexamethylene diisocyanate 33.6, benzoyl chloride 0.3, I 0.4, and 2-ethyl-1,3-hexanediol 182 parts, and stirred for 4 hr at 100° to give polyurethane (II) [58407-19-5] with 140-55° m.p., 3826 mol. weight and 11.35% latent NCO content. A mixture of polyester 100, II 34, TiO<sub>2</sub>, and butyl acrylate-2-ethylhexyl acrylate copolymer [58247-84-0] 10 parts was melted, solidified, pulverized sprayed on a metal sheet at 20-100 kV, and hardened at 160-220° to give a coating with 9 mm Erichsen deep-drawing elasticity (DIN 53 156), 37% elongation as determined with conical mandrel (ASTM D 522-41), and 3H pencil hardness (DIN 46 450).

IT 58247-83-9

(coatings, containing polyesters, electrostatic powder)

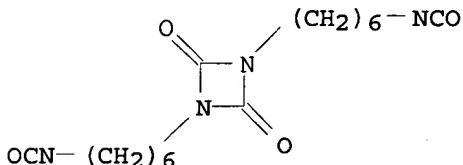
RN 58247-83-9 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatoethyl)-, polymer with 1,2-ethanediol and 2-ethyl-1,3-hexanediol (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

CMF C16 H24 N4 O4



CM 2

CRN 107-21-1

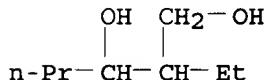
CMF C2 H6 O2

HO-CH<sub>2</sub>-CH<sub>2</sub>-OH

CM 3

CRN 94-96-2

CMF C8 H18 O2

IT 58247-81-7 58247-82-8  
(hardeners, for polyesters)

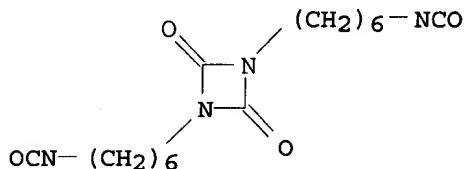
RN 58247-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with 1,4-butanediol (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

CMF C16 H24 N4 O4



CM 2

CRN 110-63-4

CMF C4 H10 O2

HO-(CH<sub>2</sub>)<sub>4</sub>-OH

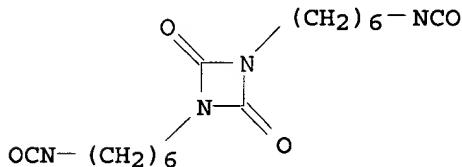
RN 58247-82-8 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

CMF C16 H24 N4 O4



IC C08G

CC 42-9 (Coatings, Inks, and Related Products)

IT 31532-63-5 58247-83-9 58407-19-5

(coatings, containing polyesters, electrostatic powder)

IT 58247-81-7 58247-82-8 58342-52-2 58383-47-4

58383-48-5 58383-49-6 58383-50-9 58383-51-0 58383-52-1

58383-53-2 58383-54-3 58383-55-4 58383-56-5

(hardeners, for polyesters)

L50 ANSWER 37 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1975:514346 HCPLUS

DOCUMENT NUMBER: 83:114346

TITLE: Triallyl isocyanurate and products from the organomagnesium compounds reactions

AUTHOR(S): Etienne, Andre; Lonchambon, Georges;

CORPORATE SOURCE: Giraudeau, Pierre; Jaubert, Bernard  
 Lab. Chim. Ind., Conservatoire Natl. Arts  
 Metiers, Paris, Fr.

SOURCE: Comptes Rendus des Seances de l'Academie des  
 Sciences, Serie C: Sciences Chimiques (1975),  
 280(15), 995-8  
 CODEN: CHDCAQ; ISSN: 0567-6541

DOCUMENT TYPE: Journal

LANGUAGE: French

OTHER SOURCE(S): CASREACT 83:114346

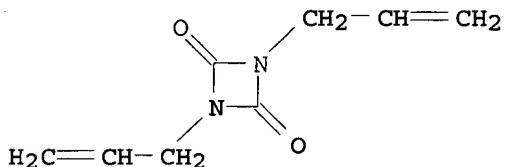
GI For diagram(s), see printed CA Issue.

AB Triallyl isocyanurate (I) was prepared by trimerizing CH<sub>2</sub>:CHCH<sub>2</sub>NCO in ClCH<sub>2</sub>CH<sub>2</sub>Cl in the presence of Bu<sub>3</sub>P. I hydrolyzed in base to 1,3,5-triallylbiuret. Reaction of I with organomagnesium halides gave the triazinols II (R = Me, Et, CH<sub>2</sub>Ph, Ph, C<sub>6</sub>H<sub>4</sub>Cl-4). II dehydrated on distillation under N to give III (X = CH<sub>2</sub>, CHMe, CHPh), which formed salts with acids.

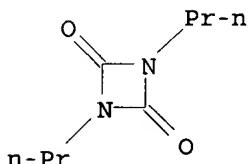
IT 23336-35-8P 56601-12-8P  
 (preparation of)

RN 23336-35-8 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-di-2-propenyl- (9CI) (CA INDEX NAME)



RN 56601-12-8 HCPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-dipropyl- (9CI) (CA INDEX NAME)



CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))  
 IT 4015-16-1P 23336-35-8P 36020-44-7P 56601-12-8P  
 56601-16-2P 56601-17-3P 56601-18-4P 56601-19-5P  
 56601-20-8P 56601-22-0P 56601-23-1P 56601-25-3P  
 56601-27-5P 56601-29-7P 56601-30-0P  
 (preparation of)  
 IT 998-40-3  
 (trimerization of allyl isocyanate in presence of)

L50 ANSWER 38 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1972:572104 HCPLUS  
 DOCUMENT NUMBER: 77:172104  
 TITLE: Phosphorothio(isocyanatidic)  
 bis(dimethylamide) and bis(diethylamide)  
 AUTHOR(S): Boden, Gisela; Grosskreutz, Werner; Kessler,  
 Gudrun; Scheler, Hermann

CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, Ger. Dem. Rep.

SOURCE: Zeitschrift fuer Chemie (1972), 12(8), 299

CODEN: ZECEAL; ISSN: 0044-2402

DOCUMENT TYPE: Journal

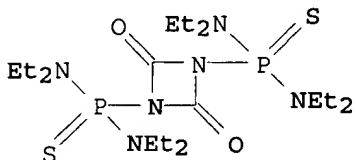
LANGUAGE: German

AB The reaction of  $(R_2N)_2P(S)Cl$  with  $AgOCN$  gave  $(R_2N)_2P(S) NCO$  [R = Me (I) or Et (II)]. I was also prepared by reaction of  $(Me_2N)_2P(S)NH_2$  (III) with  $COCl_2$ . Reaction of I with  $NH_3(g)$  gave  $(Me_2N)_2P(S)NHCONH_2$ . Reaction of II with  $2,4,5-Cl_3C_6H_2NH_2$  gave  $(Et_2N)_2P(S)NHCONHC_6H_2Cl_3-2,4,5$ . Hydrolysis of I and II gave III and  $(Et_2N)_2P(S)NH_2$ , resp. Reaction of dimeric  $(Et_2N)_2PNCO$  (IV) with S gave  $[(Et_2N)_2P(S)NCO]_2$  (V) of uretidione structure. The reaction of dimeric IV with  $SPCl_3$  gave V,  $Et_2NP(S)Cl_2$ ,  $Et_2NP(S)(NCO)_2$ , and II.

IT 38590-06-6P  
(preparation of)

RN 38590-06-6 HCPLUS

CN Phosphonothioic diamide,  $P,P'$ -(2,4-dioxo-1,3-diazetidine-1,3-diyl)bis[N,N,N',N'-tetraethyl- (9CI) (CA INDEX NAME)



CC 78-8 (Inorganic Chemicals and Reactions)

ST phosphorothioisocyanatidic diamide; isocyanatothiophosphoric diamide; thiocyanatothiophosphoric diamide; ureidothiophosphoric diamide; amide thiophosphoryl

IT 1069-08-5P 5022-58-2P 38590-03-3P 38590-05-5P  
38590-06-6P 38590-08-8P 38590-10-2P  
(preparation of)

L50 ANSWER 39 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1971:540742 HCPLUS

DOCUMENT NUMBER: 75:140742

TITLE: Di-tert-butyluretidinedione

AUTHOR(S): Stowell, John C.; Greene, Frederick D.; Bergmark, William R.

CORPORATE SOURCE: Dep. Chem., Louisiana State Univ., New Orleans, LA, USA

SOURCE: Journal of Organic Chemistry (1971), 36(20), 3056-7

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

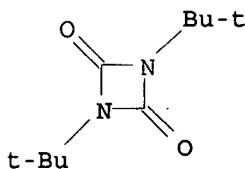
LANGUAGE: English

AB Reaction of  $Me_3CNHCONHMe_3$  with pyridine-phosgene affords di-tert-butyluretidinedione and di-tert-butylcarbodiimide. Both photolysis and thermolysis ( $200^\circ$ ) of the uretidinedione afford  $Me_3CNCO$ .

IT 30885-14-4P  
(preparation of)

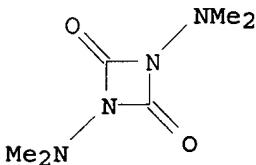
RN 30885-14-4 HCPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))  
 ST uretidinedione butyl; isocyanate butyl  
 IT 30885-14-4P  
 (preparation of)

L50 ANSWER 40 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1971:13211 HCPLUS  
 DOCUMENT NUMBER: 74:13211  
 TITLE: Silicon-nitrogen cleavage reactions in  
 N,N-dimethyl-N',N-dimethyl-N',N'-  
 bis(trimethylsilyl)hydrazine  
 AUTHOR(S): Glemser, Oskar; Kluever, Horst  
 CORPORATE SOURCE: Anorg.-Chem. Inst., Univ. Goettingen,  
 Goettingen, Fed. Rep. Ger.  
 SOURCE: Chemische Berichte (1970), 103(11), 3661-6  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB Treatment of  $\text{Me}_2\text{NN}(\text{SiMe}_3)_2$  (I) with  $\text{COF}_2$  in petroleum ether at  $-30^\circ$  to  $0^\circ$  or with  $\text{POF}_3$  in  $\text{MeCN}$  at  $-20^\circ$ , yielded  $\text{Me}_3\text{SiF}$  (II) and bis(dimethylaminoisocyanate) or  
 $\text{Me}_2\text{NN}[\text{P}(\text{O})\text{F}_2]\text{SiMe}_3$ , resp. Reaction of I with  $\text{P}_2\text{O}_3\text{F}_4$  containing  
 $\text{HOP}(\text{O})\text{F}_2$  in  $\text{Et}_2\text{O}$  at  $0^\circ$  gave  $\text{Me}_2\text{NNHP}(\text{O})\text{F}_2$  and  $\text{Me}_3\text{SiOP}(\text{O})\text{F}_2$ .  
 Heating I and  $\text{POCl}_3$  at  $80^\circ$  yielded  $\text{Me}_2\text{NN}[\text{P}(\text{O})\text{Cl}_2]_2$  and  $\text{Me}_3\text{SiCl}$ . Reaction of I and  $\text{PSF}_3$  in  $\text{MeCN}$  at  $30^\circ$  in an  
 autoclave gave  $\text{Me}_2\text{NN}[\text{P}(\text{S})\text{F}_2]\text{SiMe}_3$  and II.  
 IT 29938-12-3P  
 (preparation of)  
 RN 29938-12-3 HCPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-bis(dimethylamino)- (9CI) (CA  
 INDEX NAME)

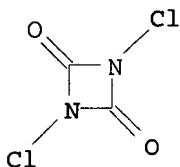


CC 29 (Organometallic and Organometalloidal Compounds)  
 IT 29938-12-3P 29938-13-4P 29938-14-5P 29938-15-6P  
 30041-94-2P  
 (preparation of)

L50 ANSWER 41 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1970:100564 HCPLUS  
 DOCUMENT NUMBER: 72:100564  
 TITLE: Chemistry of chloroisocyanate. III.

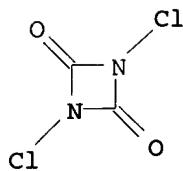
AUTHOR(S): Gottardi, W.; Henn, D.  
 CORPORATE SOURCE: Inst. Anorg. Anal. Chem., Univ. Innsbruck, Innsbruck, Austria  
 SOURCE: Monatsh. Chem. (1970), 101(1), 264-74  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German

GI For diagram(s), see printed CA Issue.  
 AB The phys. and chemical properties of 1,3-dichlorouretidine-2,4-dione (I) (ibid., 1969) are described. Upon heating, I gave, depending on the conditions, ClNCO, Cl<sub>2</sub>NCONCO, or 1,3,5-trichloro-2,4,6-trioxohexahydro-s-triazine. The reaction of I with EtOH gave ClNHCONHCO<sub>2</sub>Et and H<sub>2</sub>NCONHCO<sub>2</sub>Et.  
 IT 24604-62-4P (preparation of)  
 RN 24604-62-4 HCPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-dichloro- (9CI) (CA INDEX NAME)



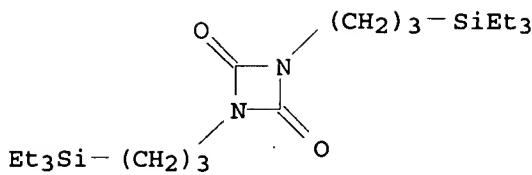
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))  
 ST chloro uretidinone; uretidinone chloro; isocyanate  
 chloro dimer; dimer isocyanate chloro; uretidinediones  
 IT 14628-80-9P 24604-62-4P 26231-93-6P 26231-94-7P  
 26231-96-9P (preparation of)

L50 ANSWER 42 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1970:67449 HCPLUS  
 DOCUMENT NUMBER: 72:67449  
 TITLE: Chemistry of chlorine isocyanate.  
 1. Polymerization, thermal behavior, and photolysis  
 AUTHOR(S): Gottardi, W.; Henn, D.  
 CORPORATE SOURCE: Inst. Anorg. Anal. Chem., Univ. Innsbruck, Innsbruck, Austria  
 SOURCE: Monatsh. Chem. (1969), 100(6), 1860-7  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB Liquid ClNCO polymerized on standing at 50° to 1,3-dichlorouretidine, trimers, and low polymers. ClNCO(g) was stable in the dark at normal pressures and temps., and at reduced pressures and elevated temps. ClNCO was extremely sensitive to photolysis, decomposing to Cl<sub>2</sub>CO, N, CO, and Cl<sub>2</sub>CONCO. The possibility of storing ClNCO and using it synthetically were discussed.  
 IT 24604-62-4P (preparation of)  
 RN 24604-62-4 HCPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-dichloro- (9CI) (CA INDEX NAME)



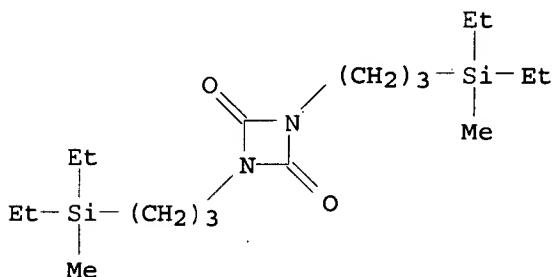
CC 35 (Synthetic High Polymers)  
 ST chlorine **isocyanate** thermolysis photolysis;  
**isocyanate** chlorine thermolysis photolysis; thermolysis  
 photolysis chlorine **isocyanate**; photolysis thermolysis  
 chlorine **isocyanate**  
 IT Ring closure  
 (in oligomerization, of chlorine **isocyanate**)  
 IT Photolysis  
 (of chlorine **isocyanate**)  
 IT Polymerization  
 (oligomerization, of chlorine **isocyanate**)  
 IT 24604-62-4P 27341-09-9P  
 (preparation of)

L50 ANSWER 43 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1970:31905 HCAPLUS  
 DOCUMENT NUMBER: 72:31905  
 TITLE: Carbofunctional organosilicon compounds. VI.  
 Uretidinedione derivatives of  
**isocyanates**  
 AUTHOR(S): Smetankina, N. P.; Miryan, N. I.; Didkovskii,  
 V. E.  
 CORPORATE SOURCE: Inst. Khim. Vysokomol. Soedin., Kiev, USSR  
 SOURCE: Zhurnal Obshchey Khimii (1969), 39(9), 2016-20  
 CODEN: ZOKHA4; ISSN: 0044-460X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB Heating 14 g Cl(CH<sub>2</sub>)<sub>3</sub>SiEt<sub>3</sub> (I) with 11.8 g KOCN in dry  
 Me<sub>2</sub>NCHO with 0.12 g Et<sub>4</sub>NI 10 min at 145° under argon gave  
 37% Et<sub>3</sub>Si(CH<sub>2</sub>)<sub>3</sub>NCO and 41.6% its dimer, b<sub>1</sub> 167-70°, n<sub>20D</sub>  
 1.4875. Similarly were prepared the dimers [R<sub>3</sub>Si(CH<sub>2</sub>)<sub>n</sub>NCO]<sub>2</sub> in  
 25-50% yields (R<sub>3</sub> and n shown); Me<sub>3</sub>, 1, b<sub>5</sub> 153°, Et<sub>3</sub>, 1,  
 b<sub>0.06</sub> 172-4°, 1.48 80; Me<sub>3</sub>, 3, b<sub>0.015</sub>  
 120°, 14610; Ph<sub>3</sub>, 3, b<sub>0.04</sub> 160-2°, 1.4800;  
 and MeEt<sub>2</sub>, 3, undistd. Heating 2 g I with 1.6 g KOCN  
 and 0.08 g Et<sub>4</sub>NI in Me<sub>2</sub>NCHO 1.5 hr at 150° in argon atmospheric  
 gave 70% above dimer. Ir spectral curves were shown. Thus, the  
 haloalkylsilanes in reacting with KOCN yield not only the  
**isocyanates** but polymers with ring systems in the chain.  
 The NCO group band in the **isocyanates** of Si lay in the  
 2270 cm<sup>-1</sup> region, while the 1690 cm<sup>-1</sup> band is that of the CO group  
 of the uretidinedione ring of the above dimers.  
 IT 24602-17-3P 24602-19-5P 24602-21-9P  
 24602-22-0P 24602-23-1P  
 (preparation of)  
 RN 24602-17-3 HCAPLUS  
 CN 2,4-Uretidinedione, 1,3-bis[3-(triethylsilyl)propyl]- (8CI) (CA  
 INDEX NAME)



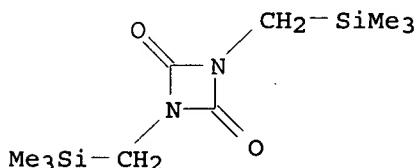
RN 24602-19-5 HCAPLUS

CN 2,4-Uretidinedione, 1,3-bis[3-(diethylmethylsilyl)propyl]- (8CI) (CA INDEX NAME)



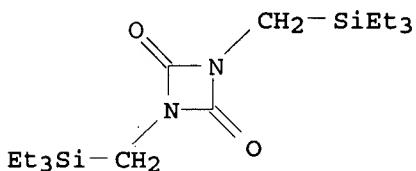
RN 24602-21-9 HCAPLUS

CN 2,4-Uretidinedione, 1,3-bis[(trimethylsilyl)methyl]- (8CI) (CA INDEX NAME)



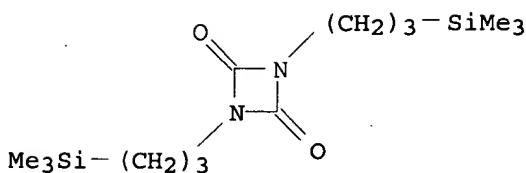
RN 24602-22-0 HCAPLUS

CN 2,4-Uretidinedione, 1,3-bis[(triethylsilyl)methyl]- (8CI) (CA INDEX NAME)



RN 24602-23-1 HCAPLUS

CN 2,4-Uretidinedione, 1,3-bis[3-(trimethylsilyl)propyl]- (8CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)  
 ST silyl isocyanate dimers; isocyanate dimers  
 silyl; dimers silyl isocyanate; uretidinediones silyl  
 IT 7440-21-3DP, Silicon, organic carbonyl derivs. 24602-17-3P  
 24602-18-4P 24602-19-5P 24602-20-8P  
 24602-21-9P 24602-22-0P 24602-23-1P  
 26246-60-6P  
 (preparation of)

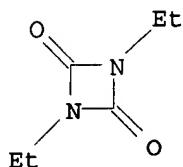
L50 ANSWER 44 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:481328 HCPLUS  
 DOCUMENT NUMBER: 71:81328  
 TITLE: Uretidinediones with aliphatic substituents  
 PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.  
 SOURCE: Fr., 6 pp.  
 CODEN: FRXXAK  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

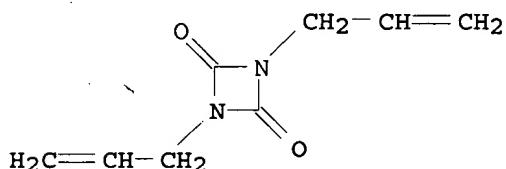
| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------|
| FR 1532054             |      | 19680705 | FR              |      |
| DE 1670720             |      |          | DE              |      |
| GB 1153815             |      |          | GB              |      |
| PRIORITY APPLN. INFO.: |      |          | DE              |      |
|                        |      |          |                 | 1966 |
|                        |      |          |                 | 0721 |

GI For diagram(s), see printed CA Issue.  
 AB Substituted uretidinediones (I) are prepared by the dimerization at 60-140° of aliphatic isocyanates in the presence of a tertiary phosphine having ≥1 aliphatic substituent or  $\text{BF}_3$  catalyst in an organic solvent and interrupting the reaction after 5-50% conversion, isolating I, and returning unreacted isocyanates to the reaction mixture. Thus, 657 parts freshly distilled  $\text{BuNCO}$  was heated at 60° with 9.85 parts  $\text{Bu}_3\text{P}$  for 4 hrs. or until a NCO content of 35.6% was obtained, the reaction stopped by adding 6.3 g.  $\text{Me}_2\text{SO}_4$ , and the mixture heated at 80° to give 16.5% conversion, and the mixture fractionated at 1.2 mm. to give 546 parts  $\text{BuNCO}$  in the cold trap and forecut (b. 45-92°) 3.6, I (R = Bu) (b. 92-3°) 49.0, intermediate fraction (b. 94-154°) 1.9, isocyanurate (b. 155-8°) 40.7, and residue 13.0 parts. Similarly prepared were the following I (R and b.p./mm. given): Et, 73-4°/760, allyl, 66°/1.0;  $\text{MeOCH}_2$ , 86°/1.0; 6-chlorohexyl, -; 5-(isocyanatomethyl)-3,3,5-trimethylcyclohexylmethyl, -. 1,6-Hexamethylene diisocyanate uretidinedione was also prepared

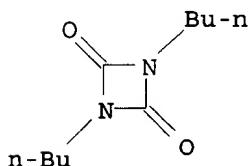
IT 23336-34-7P 23336-35-8P 23336-44-9P  
 23336-45-0P 23336-46-1P 23501-81-7P  
 (preparation of)  
 RN 23336-34-7 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-diethyl- (9CI) (CA INDEX NAME)



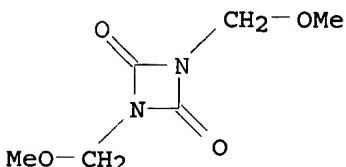
RN 23336-35-8 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-di-2-propenyl- (9CI) (CA INDEX NAME)



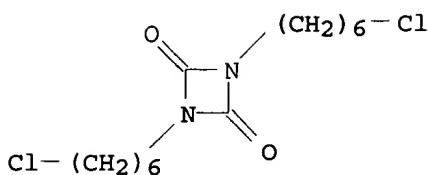
RN 23336-44-9 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-dibutyl- (9CI) (CA INDEX NAME)



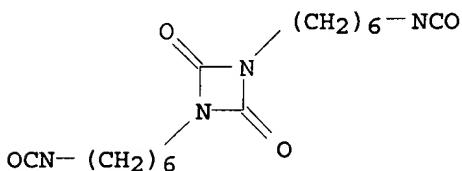
RN 23336-45-0 HCAPLUS  
 CN 2,4-Uretidinedione, 1,3-bis(methoxymethyl)- (8CI) (CA INDEX NAME)



RN 23336-46-1 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-chlorohexyl)- (9CI) (CA INDEX NAME)



RN 23501-81-7 HCAPLUS  
 CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA  
 INDEX NAME)



IC C07D  
 CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))  
 ST **isocyanates** dimerization; dimerization  
**isocyanates**; uretidinediones from **isocyanates**  
 IT 715-63-9P 846-74-2P 1025-15-6P 17576-39-5P 21132-72-9P  
 23336-34-7P 23336-35-8P 23336-44-9P  
 23336-45-0P 23336-46-1P 23370-68-5P  
 23501-78-2P, s-Triazine-2,4,6(1H,3H,5H)-trione,  
 1,3,5-tris(methoxymethyl)- 23501-81-7P 23544-79-8P  
 (preparation of)

L50 ANSWER 45 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:75614 HCAPLUS

DOCUMENT NUMBER: 66:75614

TITLE: Preparation and properties of  
 chlorofluoromethylsulfenyl pseudohalides

AUTHOR(S): Haas, Alois; Oh, Dong-Young

CORPORATE SOURCE: Univ. Goettingen, Goettingen, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1967), 100(2), 480-91

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

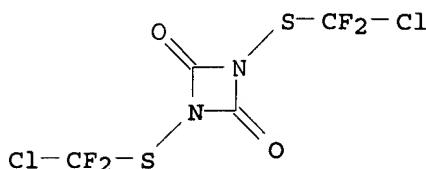
LANGUAGE: German

OTHER SOURCE(S): CASREACT 66:75614

AB C12FCSCl (I) and C1F2CSCl (II) without solvent gave with AgOCN the corresponding monomeric **isocyanates** but in C6H6 the **isocyanurates** were formed. The hydrolysis and alcoholysis of the **isocyanates** is described. C1F2CSNCO dimerized slowly at 20° to the corresponding uretidinedione. I and II with AgSCN yielded C12FCSSCN and C1F2CSSCN, resp., which decomposed readily to (C12FCS)2 and (C1F2CS)2, resp., and (SCN)x. The ir and 19F N.M.R. spectra of the new compds. are discussed. Gradual differences in the phys. and chemical properties were observed in the course of the reaction and in the behavior of the compds. with increasing degree of fluorination. Characteristic ir bands were assigned to the groups C12FCS and C1F2CS; these bands and the 19F chemical shifts can be used for the identification.

IT 14674-07-8P  
 (preparation of)

RN 14674-07-8 HCPLUS  
 CN 2,4-Uretidinedione, 1,3-bis[(chlorodifluoromethyl)thio]- (8CI)  
 (CA INDEX NAME)



CC 23 (Aliphatic Compounds)  
 ST NMR SULFENYL PSEUDOHALIDES; CHLOROFLUOROMETHYLSULFENYL  
 PSEUDOHALIDES; IR SULFENYL PSEUDOHALIDES; SULFENYL PSEUDOHALIDES;  
 PSEUDOHALIDES CHLOROFLUOROMETHYLSULFENYL; ISOCYANATES;  
 ISOCYANURATES; URETIDINEDIONES  
 IT 692-58-0P 14673-88-2P 14673-90-6P 14673-91-7P 14673-92-8P  
 14673-93-9P 14674-05-6P 14674-06-7P 14674-07-8P  
 14674-08-9P 14999-95-2P 15085-84-4P  
 (preparation of)

L50 ANSWER 46 OF 46 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:18702 HCPLUS

DOCUMENT NUMBER: 66:18702

TITLE: Thioacyl isocyanates. V.

Substituted thiazoline-4,5-diones and their  
 thermal cleavage into isocyanates  
 and mustard oils

AUTHOR(S): Goerdeler, Joachim; Jonas, Klaus

CORPORATE SOURCE: Univ. Bonn, Bonn, Germany

SOURCE: Chemische Berichte (1966), 99(11), 3572-81

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 66:18702

GI For diagram(s), see printed CA Issue.

AB cf. CA 64, 19456d. A series of 2-X substituted  
 4,5-dihydro-4,5-dioxothiazoles (I) with functional groups in the  
 2-position was prepared and converted thermally into the  
 corresponding XC(:S)NCO (II). The II were either isolated as such  
 or captured with amines or PhCH:NPh. The dimerization of the II  
 gave 6-(X substituted)-3-[C(:S)X substituted] 2,3-dihydro-4H-1,3,5-  
 thiadiazine-2,4-diones (III) and in 1 case the  
 N,N'-bis(-thionopyruvyl)analog (IV) of diazetidinedione. All  
 isocyanates rearranged thermally to the corresponding  
 XC(O)NCS; the rate of the rearrangement showed clearly substituent  
 dependence. Me<sub>2</sub>NCSNH<sub>2</sub> (1 g.) and 3.3 cc. Et<sub>3</sub>N in 150 cc. AcOEt  
 and 1 cc. (COCl)<sub>2</sub> in 30 cc. AcOEt added simultaneously dropwise  
 with stirring at -30° to 100 cc. dry AcOEt and warmed to  
 4° yielded 0.8 g. yellow I (X = Me<sub>2</sub>N), m. 190°  
 (decomposition) (repptd. from dry CHCl<sub>3</sub> with petroleum ether).  
 Similarly were prepared the following I (X, m.p. with decomposition, and  
 % yield given): Et<sub>2</sub>N, 90° (repptd. from C<sub>6</sub>H<sub>6</sub> with petroleum  
 ether), 71; piperidino (V), 126° (AcOEt), 73; MePhN,  
 140° (repptd. from CHCl<sub>3</sub> with petroleum ether), 73; EtPhN  
 (VI), 160° (repptd. from CHCl<sub>3</sub> with petroleum ether), 75;  
 BuPhN, 118° (petroleum ether-AcOEt), 65. The appropriate  
 O-alkyl or aryl thiocarbamate in CH<sub>2</sub>Cl<sub>2</sub> and an equivalent amount (COCl)<sub>2</sub>

in  $\text{CH}_2\text{Cl}_2$  added dropwise simultaneously at  $0^\circ$  dropwise during about 0.5 hr. to dry  $\text{CH}_2\text{Cl}_2$  or  $(\text{CH}_2\text{Cl})_2$  and evaporated rapidly yielded the corresponding I. In this manner were prepared the following I (X, m.p., and % yield given):  $\text{MeO}$ ,  $118^\circ$  (decomposition) (reptd. from  $\text{C}_6\text{H}_6$  with petroleum ether), 69;  $\text{EtO}$ ,  $44-6^\circ$  (petroleum ether), 65;  $\text{PhO}$  (VII),  $118-20^\circ$  (decomposition), 72; cyclohexyloxy (VIII),  $97^\circ$  (decomposition) (reptd. from  $\text{C}_6\text{H}_6$  with petroleum ether), 52.  $\text{H}_2\text{NCS}_2\text{Me}$  (1.1 g.) in 20 cc.  $\text{CH}_2\text{Cl}_2$  and 1 cc.  $(\text{COCl})_2$  in 20 cc.  $\text{CH}_2\text{Cl}_2$  added to 30 cc.  $\text{CH}_2\text{Cl}_2$  at  $0^\circ$  gave 1.2 g. canary-yellow I (X =  $\text{MeS}$ ) (IX), m.  $108^\circ$  (decomposition).  $\text{O-Cyclohexyl thiocarbamate}$  (1.6 g.) in 15 cc.  $\text{CH}_2\text{Cl}_2$  and 1 cc.  $(\text{COCl})_2$  in 15 cc.  $\text{CH}_2\text{Cl}_2$  added dropwise simultaneously at  $0^\circ$  to 15 cc.  $\text{CH}_2\text{Cl}_2$  gave 1.1 g. thiazolidine-2,4,5-trione, m.  $158^\circ$ . The appropriate I and stainless steel spirals distilled in vacuo into a receiver cooled at  $-60^\circ$  gave the corresponding II (X, m.p.,  $\text{nd/ temp}$ , temperature, and pressure in mm. Hg given):  $\text{MeO}$  (X), -, 1.498/24°, 63,  $120^\circ$ ,  $120^\circ$ ;  $\text{EtO}$  (XI), -, 1.492/19°, 67,  $110^\circ$ , 14;  $\text{PhO}$ , -24 to  $-22^\circ$ , 1.500/20°, 86,  $135^\circ$ , 0.4; cyclohexyloxy, about  $30^\circ$ , 1.520/16°, 77,  $120^\circ$ , 0.4;  $\text{MeS}$ , -22 to  $-20^\circ$ , -, 78,  $120^\circ$ , 14. XI kept 3 days at  $-20^\circ$  in a little  $\text{C}_6\text{H}_6$ , diluted with petroleum ether, and cooled to  $-30^\circ$  gave nearly quant. III (X =  $\text{EtO}$ ), m.  $80^\circ$  (decomposition). Similarly were prepared the following III in nearly quant. yields (X, m.p., reaction temperature, and reaction time given): cyclohexyloxy,  $90-100^\circ$  (decomposition), room temperature, 30 hrs.;  $\text{PhO}$ , about  $140^\circ$ , room temperature, 15 min.;  $\text{MeS}$ ,  $142^\circ$  (decomposition),  $-20^\circ$ , overnight. Crystalline V (1 g.) kept 3 min. at  $140^\circ$  in vacuo and cooled to  $0^\circ$  gave 0.4 g. III (X = piperidino) (XII), m.  $160^\circ$  (decomposition). X kept 20 hrs. at  $-60$  to  $-20^\circ$  and the product reptd. from  $\text{AcOEt}$  with petroleum ether at  $0^\circ$  gave nearly 100% IV, m.  $170^\circ$  (decomposition). The appropriate I (2.5 millimoles) and 0.45 g.  $\text{PhCH:NPPh}$  in 10 cc.  $\text{MePh}$  heated 4 min. at  $100^\circ$  gave the corresponding 2,3,5,6-tetrahydro-4H-2-(X-substituted)-6-phenyl-1,3,5-thiadiazin-4-ones (XIII) (X, m.p. with decomposition, and % yield given):  $\text{EtPhN}$ ,  $170-5^\circ$ , 93;  $\text{MeO}$ ,  $160^\circ$ ; 94;  $\text{PhO}$ ,  $140-50^\circ$ , 95; cyclohexyloxy,  $180-90^\circ$ , 76;  $\text{Ph}_2\text{N}$ ,  $170-5^\circ$ , 90. XII (0.4 g.) and 0.35 g.  $\text{p-O}_2\text{NC}_6\text{H}_4\text{NH}_2$  in 40 cc.  $\text{MePh}$  kept 5 hrs. at  $60^\circ$  yielded 0.4 g. beige XC(:S) $\text{NHCONHAr}$  (XIV) (X = piperidino, Ar =  $\text{p-O}_2\text{NC}_6\text{H}_4$ ), m.  $204^\circ$  (decomposition). 2-Diphenylaminothiazoline-4,5-dione (0.35 g.) in 10 cc.  $\text{MePh}$  heated 3 min. at  $100^\circ$ , cooled to  $0^\circ$ , treated with 0.15 g.  $\text{PhNH}_2$ , and kept 1 hr. at room temperature gave 0.25 g. XIV (X =  $\text{Ph}_2\text{N}$ , Ar = Ph), m.  $135-7^\circ$  (decomposition) (petroleum ether). I (X =  $\text{MeO}$ ) (0.35 g.) and 0.25 g.  $\text{PhNH}_2$  gave similarly 0.5 g. XIV (X =  $\text{MeO}$ , Ar = Ph). VII (0.5 g.) and 0.25 g.  $\text{PhNH}_2$  gave similarly during 0.5 hr. at room temperature 0.65 g. XIV (X =  $\text{PhO}$ , Ar = Ph), m.  $182-4^\circ$  (decomposition) (ligroine, b.  $100-40^\circ$ ). VIII (0.5 g.) in 15 cc.  $\text{MePh}$  kept 4 min. at  $100^\circ$ , cooled to  $0^\circ$ , and treated with 2.5 g.  $\text{PhNH}_2$  gave 0.6 g. XIV (X = cyclohexyloxy, Ar = Ph), m.  $136^\circ$  (ligroine). II (X =  $\text{MeS}$ ) (1.3 g.) and 0.9 g.  $\text{PhNH}_2$  gave similarly 2.15 g. XIV (X =  $\text{MeS}$ , Ar = Ph), m.  $200-5^\circ$  (decomposition) (ligroine). V (0.5 g.) in 100 cc.  $\text{MePh}$  kept 20 min. at  $100^\circ$ , cooled to room temp., and treated 1 hr. with 0.25 g.  $\text{PhNH}_2$  yielded 0.6 g. N-piperidinoformyl-N'-phenylthiourea (XV), m.  $125^\circ$  (decomposition) (ligroine). V (0.5 g.) and 0.35 g.  $\text{p-O}_2\text{NC}_6\text{H}_4\text{NH}_2$  gave

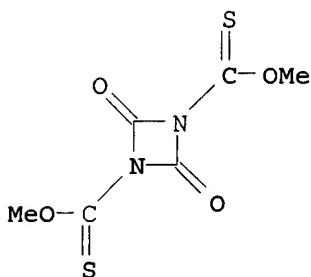
similarly at room temperature during 2 hrs. 0.6 g. beige p-NO<sub>2</sub> derivative of XV, m. 152° (decomposition) (EtOH). VI (0.6 g.) with 0.35 g. p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> gave similarly 0.7 g. p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NHCSNHO<sub>2</sub>CNETPh, m. 180° (decomposition) (Me<sub>2</sub>CO). IX (0.4 g.) and 0.25 g. PhNH<sub>2</sub> yielded 0.45 g. MeSCONHCSNPh, m. 168° (decomposition) (petroleum ether-AcOEt).

IT 13163-42-3P

(preparation of)

RN 13163-42-3 HCAPLUS

CN 1,3-Uretidinedicarbothioic acid, 2,4-dioxo-, O,O'-dimethyl ester (8CI) (CA INDEX NAME)



CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))

ST ISOCYANATES THIOACYL; THIAZOLINEDIONES; MUSTARD OILS;

THIOACYL ISOCYANATES; THIAZOLINEDIONES;

ISOCYANATES THIOACYL; THIOACYL ISOCYANATES;

MUSTARD OILS

IT Allophanic acid, 4-phenyl-1,3-dithio-, S-methyl ester

Biuret, 1,1,5-triphenyl-2-thio-

Carbonic acid, dithio-, monoanhydride with isocyanic acid, S-methyl ester

Carbonic acid, dithio-, monoanhydride with isocyanic acid, S-methyl ester

Formic acid, isocyanatothiobis-, methyl ester

(preparation of)

IT 5729-32-8P 13163-09-2P 13163-10-5P 13163-11-6P 13163-12-7P

13163-13-8P 13163-20-7P 13163-31-0P 13163-32-1P

13163-33-2P 13163-34-3P 13163-35-4P 13163-36-5P, Isocyanic acid, anhydride with S-methyl dithiocarbonate 13163-36-5P

13163-37-6P 13163-38-7P 13163-39-8P 13163-40-1P

13163-41-2P 13163-42-3P 13163-43-4P 13163-44-5P

13163-45-6P 13163-46-7P 13163-47-8P 13163-49-0P

13163-50-3P 13163-51-4P 13163-52-5P 13163-53-6P

13163-54-7P 13332-83-7P 13332-84-8P 13332-85-9P

13332-86-0P 13332-87-1P 13559-72-3P

(preparation of)